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(54)	POLYCARBONATE COMPOSITIONS HAVING
, ,	ENHANCED OPTICAL PROPERTIES,
	METHODS OF MAKING AND ARTICLES
	COMPRISING THE POLYCARBONATE
	COMPOSITIONS

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CPC . **C08G 64/24** (2013.01); **C08J 5/18** (2013.01); **C08L 69/00** (2013.01); **C08J 2369/00** (2013.01); **H01L 33/56** (2013.01)

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## 57) ABSTRACT

In some embodiments, a composition comprises a bisphenol-A polycarbonate, wherein a molded article of the composition has transmission level greater than or equal to 90.0% at 2.5 mm thickness as measured by ASTM D1003-00 and a yellow index (YI) less than or equal to 1.5 as measured by ASTM D1925.

## 13 Claims, 7 Drawing Sheets

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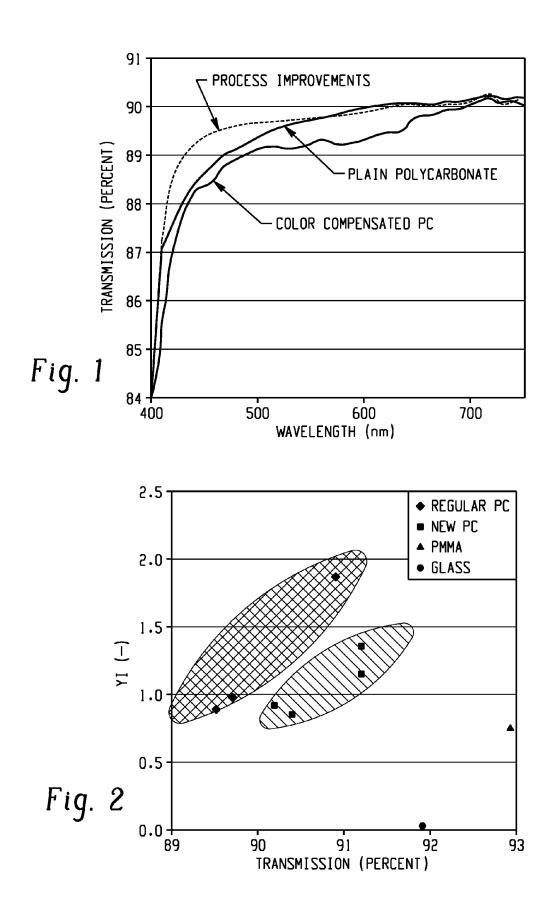
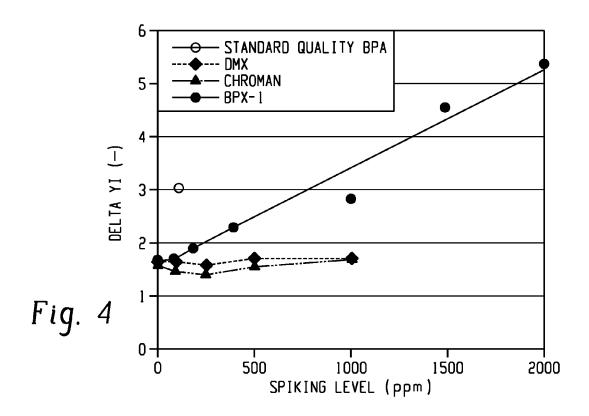
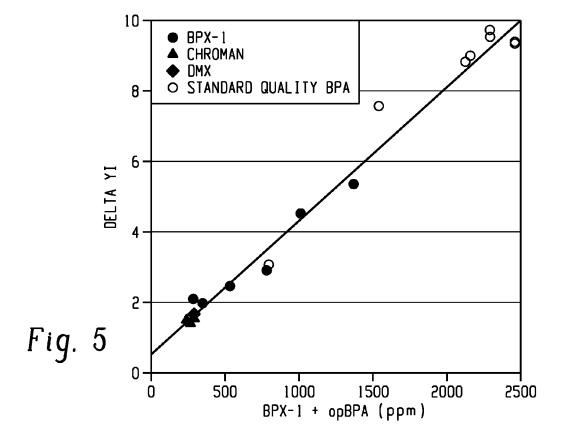
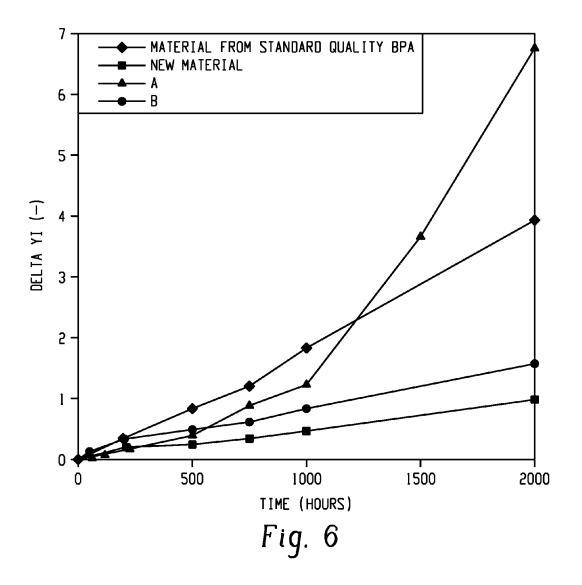


Fig. 3







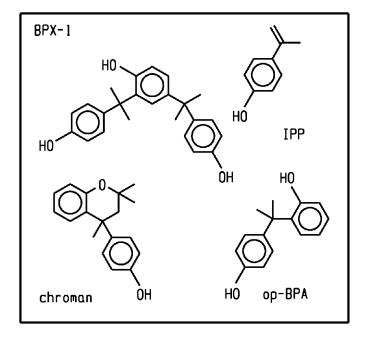
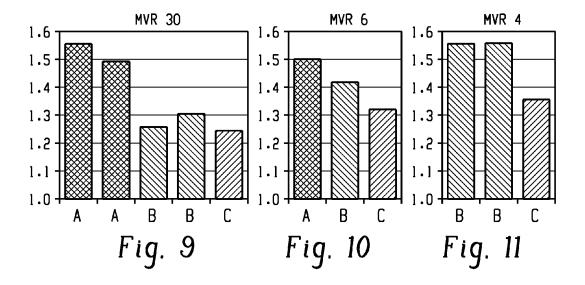


Fig. 8



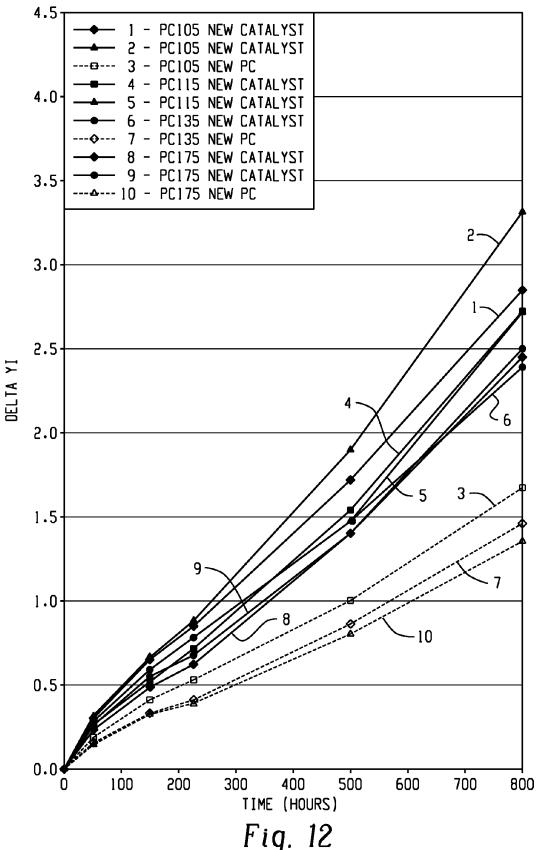


Fig. 12

PEPQ

Fig. 13

# POLYCARBONATE COMPOSITIONS HAVING ENHANCED OPTICAL PROPERTIES, METHODS OF MAKING AND ARTICLES COMPRISING THE POLYCARBONATE COMPOSITIONS

# CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims the benefit of U.S. Patent Applica-  $^{10}$ tion No. 61/515,365, filed Aug. 5, 2011, which is incorporated by reference in its entirety herein.

#### BACKGROUND

The present disclosure generally relates to polycarbonate compositions, and more particularly, to polycarbonate compositions having enhanced optical properties, methods of manufacture, and uses thereof.

Polycarbonate is a high-performance plastic with good 20 impact strength (ductility). Polycarbonates, however, can age under the influence of heat, light, and time, causing reduced light transmission and color changes.

There accordingly remains a need for polycarbonate compositions having enhanced optical properties, methods of 25 for an exemplary polycarbonate (LEXAN\* polycarbonate making and articles comprising the polycarbonate compositions.

#### **BRIEF DESCRIPTION**

Disclosed herein are polycarbonate compositions having enhanced optical properties, methods for making the polycarbonate composition, and articles comprising the polycarbonate compositions.

In one embodiment, a composition comprises a bisphe- 35 nol-A polycarbonate, wherein a molded article of the composition has transmission level greater than or equal to 90.0% at 2.5 mm thickness as measured by ASTM D1003-00 and a yellow index (YI) less than or equal to 1.5 as measured by ASTM D1925.

In another embodiment, a method of making a polycarbonate composition comprises polymerizing, by an interfacial polymerization, reactants comprising a starting material, the starting material comprising a bisphenol-A having a purity of greater than or equal to 99.65 wt % and a sulfur content of less 45 than or equal to 2 ppm. The polycarbonate composition has a free hydroxyl content of less than or equal to 150 ppm, and a molded article of the polycarbonate composition has transmission level greater than or equal to 90.0% at 2.5 mm thickness as measured by ASTM D1003-00 and a yellow index 50 (YI) less than or equal to 1.5 as measured by ASTM D1925.

These and other non-limiting characteristics are more particularly described below.

# BRIEF DESCRIPTION OF DRAWINGS

FIG. 1 is a graph depicting transmission (%) versus wavelength (nanometers (nm)) of polycarbonates.

FIG. 2 is a graph depicting the yellowness and transmission of polycarbonate (PC) compared to PMMA (polymethyl 60 methacrylate) and standard uncoated glass (yellowness index (YI(-)) versus transmission (%)).

FIG. 3 is a schematic illustration of selected BPA impurities potentially related to color.

FIG. 4 is a graph depicting changes in YI after 2000 hours, 65 heat aging at 130° C. as a function of spiking level of three different impurities (delta YI(-) versus spiking level (ppm)).

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FIG. 5 is a graph depicting the change in YI after 2,000 hours, heat aging at 130° C. as a function of the summed level of BPX-1 and opBPA as determined analytically (delta YI versus BPX-1+opBPA (ppm).

FIG. 6 is a graph depicting implementation of the described process improvements combined with an optimized formulation improved the polycarbonate (PC) grade beyond comparison performance (delta YI(-) versus time (hours)).

FIG. 7 is an exemplary chemical formula illustrating the formation of BPA.

FIG. 8 is an example of an exemplary bound catalyst (attached to an insoluble resin for the reduction of sulfur in BPA.

FIG. 9 is a bar graph comparing the yellowness index (YI) for an exemplary polycarbonate (LEXAN\* polycarbonate grade PC175 having a melt volume rate of 30) with the bulk catalyst ("A"), the attached catalyst ("B"), and with the attached catalyst and a BPA purity of 99.65 wt % ("C").

FIG. 10 is a bar graph comparing the yellowness index (YI) for an exemplary polycarbonate (LEXAN\* polycarbonate grade PC105 having a melt volume rate of 6) with the bulk catalyst ("A"), the attached catalyst ("B"), and with the attached catalyst and a BPA purity of 99.65 wt % (also referred to as "new BPA" "C").

FIG. 11 is a bar graph comparing the yellowness index (YI) grade PC135 having a melt volume rate of 4) with the attached catalyst ("B"), and with the attached catalyst and a BPA purity of 99.65 wt % ("C").

FIG. 12 is a graphical illustration of change in YI over time for various grades of LEXAN\* polycarbonate formed with the new catalyst or with the new BPA using a free hydroxyl concentration of less than 150 ppm.

FIG. 13 is various chemical structures for materials discussed herein.

#### DETAILED DESCRIPTION

According to embodiments, polycarbonate compositions having enhanced optical properties are disclosed, as well as 40 their methods of manufacture and uses thereof, and articles made therefrom.

In accordance with an embodiment, and as further described below, the inventors have developed an interfacial process to manufacture a composition comprising a polycarbonate, such as a BPA polycarbonate, with transmission levels higher than 90.0% at 2.5 millimeter (mm) thickness, and a YI lower than 1.5, with an increase in YI of less than 2 during 2,000 hours of heat aging at 130° C. As used herein, YI is measured in accordance with ASTM D1925, while transmission is measured in accordance with ASTM D-1003-00, Procedure A, measured, e.g., using a HAZE-GUARD DUAL from BYK-Gardner, using and integrating sphere (0°/diffuse geometry), wherein the spectral sensitivity conforms to the International Commission on Illumination (CIE) standard 55 spectral value under standard lamp D65.

The enhanced optical properties can be achieved by employing in the interfacial process a starting BPA monomer having both an organic purity (e.g., measured by HPLC of greater than or equal to 99.65 wt %) and a sulfur level of less than or equal to 2 ppm. The organic purity can be defined as 100 wt % minus the sum of known and unknown impurities detected using ultraviolet (UV) (see HPLC method in Nowakowska et al., Polish J. Appl. Chem., XI(3), 247-254 (1996)). The use of an end-capping agent can be employed in the reaction such that the resultant composition comprising BPA polycarbonate comprises a free hydroxyl level less than or equal to 150 ppm. Also, the sulfur level in the resultant composition (resin) can be less than or equal to 2 ppm, as measured by a commercially available Total Sulfur Analysis based on combustion and coulometric detection.

It has been discovered that a surprising synergist effect can be achieved resulting in enhanced optical qualities (e.g., transmission levels higher than 90.0% at 2.5 mm thickness and a YI less than or equal to 1.5) by reacting, in an interfacial process (as opposed to a melt process), a low sulfur (less than or equal to 2 ppm) and highly pure (purity greater than or equal to 99.65 wt %) BPA starting material to form a BPA polycarbonate comprising a free hydroxyl level of less than or equal to 150 ppm.

The disclosed interfacial process enhances the optical properties of BPA polycarbonate (e.g., Lexan\* polycarbonate), upgrading transparency and improving the durability of this transparency by lowering the blue light absorption.

While various types of polycarbonates could potentially be used in accordance with embodiments and are described in detail below, of particular interest are BPA polycarbonates,  $_{20}$ such as Lexan\* polycarbonate (Lexan\* is a trademark of SABIC Innovative Plastics IP B. V.). More particularly, according to embodiments, Lexan\* polycarbonate can be used for a wide range of applications that make use of its interesting combination of mechanical and optical properties. 25 wherein at least 60 percent of the total number of R1 groups Its high impact resistance can make it an important component in numerous consumer goods such as mobile phones, MP3 players, computers, laptops, etc. Due to its transparency, this BPA polycarbonate can find use in optical media, automotive lenses, roofing elements, greenhouses, photovoltaic devices, and safety glass. The developments in light emitting diode (LED) technology have led to significantly prolonged lifetimes for the lighting products to which this technology can be applied. This has led to increased requirements on the 35 durability of polycarbonates, in particular on its optical properties. In other applications such as automotive lighting, product developers may feel the need to design increasingly complex shapes which cannot be made out of glass and for which the heat requirements are too stringent for polymethyl methacrylate (PMMA). Also in these applications polycarbonate is the material of choice, but the high transparency of PMMA and glass should be approached as closely as possible.

Polycarbonate has the tendency to develop a yellow tint 45 due to light absorption stretching into the blue regions of the spectrum (FIG. 1, line-R); a tint which gets worse upon heat aging. FIG. 1 is a graph depicting transmission spectra of polycarbonates (transmission (%) versus wavelength (nm)). This tint can be compensated for through the addition of 50 colorants which absorb light in the yellow region to give a neutral tint (FIG. 1, line-B). Absorbing blue and yellow light lowers the overall transmission of the material, see FIG. 2. FIG. 2 is a graph depicting the yellowness and transmission of PC compared to PMMA and standard uncoated glass (YI(-) 55 versus transmission (%)). With colorants, it is possible to move within one of the ellipsoid areas, lowering yellowness at the expense of transmission. By making process improvements, one can move from the darker area to the lighter one, lowering yellowness while gaining transmission. The inventors have determined that it would thus be desirable to have a colorless material by preventing or removing the blue light absorption which will increase the overall transmission (FIG. 1, dotted line-G).

As noted above, although BPA polycarbonates, such as 65 Lexan\* polycarbonates are of particular interest, various polycarbonates could potentially be employed in the embodi-

ments disclosed herein. For example, in general, various types of polycarbonates that have a repeating structural background of the following formula:

$$R^1$$
OOOOO

can be utilized for embodiments encompassed by this disclo-

The selection of a polycarbonate backbone of choice depends on many factors such as end use and other factors understood by one of ordinary skill the art.

In one embodiment, the polycarbonates have repeating structural carbonate units of the formula (1):

$$\begin{array}{c|c}
 & O \\
 & R^1 - O \\
\end{array}$$

contains aromatic organic groups and the balance thereof are aliphatic, alicyclic, or aromatic groups.

In another embodiment, the polycarbonate is derived from bisphenol-A.

In another embodiment, each R<sup>1</sup> group is a divalent aromatic group, for example derived from an aromatic dihydroxy compound of the formula (3):

$$HO-A^1-Y^1-A^2-OH$$
 (3)

wherein each of A<sup>1</sup> and A<sup>2</sup> is a monocyclic divalent arylene group, and Y<sup>1</sup> is a single bond or a bridging group having one or two atoms that separate A<sup>1</sup> from A<sup>2</sup>. In an exemplary embodiment, one atom separates A1 from A2. In another embodiment, when each of  $A^1$  and  $A^2$  is phenylene,  $Y^1$  is para to each of the hydroxyl groups on the phenylenes. Illustrative non-limiting examples of groups of this type are -O--S, -S(O), -S(O), -C(O), methylene, cyclohexyl-methylene, 2-[2.2.1]-bicycloheptylidene, ethylidene, isopropylidene, neopentylidene, cyclohexylidene, cyclopentadecylidene, cyclododecylidene, and adamantylidene. The bridging group Y<sup>1</sup> can be a hydrocarbon group or a saturated hydrocarbon group such as methylene, cyclohexylidene, or isopropylidene.

Included within the scope of formula (3) are bisphenol compounds of general formula (4):

$$HO - X^a - X^a - Y^a -$$

wherein  $R^a$  and  $R^b$  each represent a halogen atom or a monovalent hydrocarbon group and can be the same or different; p and q are each independently integers of 0 to 4; and  $X^a$  represents a single bond or one of the groups of formulas (5) or (6):

wherein  $R^c$  and  $R^d$  are each independently hydrogen,  $C_{1-12}$  alkyl,  $C_{1-12}$  cycloalkyl,  $C_{7-12}$  arylalkyl,  $C_{1-12}$  heteroalkyl, or cyclic  $C_{7-12}$  heteroarylalkyl, and  $R^e$  is a divalent  $C_{1-12}$  hydrocarbon group. In particular,  $R^c$  and  $R^d$  are each the same hydrogen or  $C_{1-4}$  alkyl group, specifically the same  $C_{1-3}$  alkyl

group, even more specifically, methyl.

In an embodiment,  $R^c$  and  $R^d$  taken together represent a  $C_{3\text{-}20}$  cyclic alkylene group or a heteroatom-containing  $C_{3\text{-}20}$  cyclic alkylene group comprising carbon atoms and heteroatoms with a valency of two or greater. These groups can be in the form of a single saturated or unsaturated ring, or a fused polycyclic ring system wherein the fused rings are saturated, unsaturated, or aromatic. A specific heteroatom-containing cyclic alkylene group comprises at least one heteroatom with a valency of 2 or greater, and at least two carbon atoms. Exemplary heteroatoms in the heteroatom-containing cyclic alkylene group include -O-, -S-, and -N(Z)-, where Z is a substituent group selected from hydrogen, hydroxy,  $C_{1\text{-}12}$  alkyl,  $C_{1\text{-}12}$  alkoxy, or  $C_{1\text{-}12}$  acyl.

In a specific exemplary embodiment,  $X^a$  is a substituted  $C_{3-18}$  cycloalkylidene of the formula (7):

$$(R^{p}) \xrightarrow{h} (I)_{i} \xrightarrow{C} (C)_{k} \xrightarrow{-(\cdot R^{t})_{j}}$$

$$(7)$$

wherein each  $R^r$ ,  $R^p$ ,  $R^q$ , and  $R^t$  is independently hydrogen, halogen, oxygen, or  $C_{1-12}$  organic group; I is a direct bond, a carbon, or a divalent oxygen, sulfur, or -N(Z)- wherein Z is hydrogen, halogen, hydroxy,  $C_{1-12}$  alkyl,  $C_{1-12}$  alkoxy, or  $C_{1-12}$  acyl; h is 0 to 2, j is 1 or 2, i is an integer of 0 or 1, and 50 k is an integer of 0 to 3, with the proviso that at least two of  $\mathbb{R}^r$ ,  $\mathbb{R}^p$ ,  $\mathbb{R}^q$ , and  $\mathbb{R}^t$  taken together are a fused cycloaliphatic, aromatic, or heteroaromatic ring. It will be understood that where the fused ring is aromatic, the ring as shown in formula (7) will have an unsaturated carbon-carbon linkage where the 55 ring is fused. When k is 1 and i is 0, the ring as shown in formula (7) contains 4 carbon atoms, when k is 2, the ring as shown contains 5 carbon atoms, and when k is 3, the ring contains 6 carbon atoms. In one embodiment, two adjacent groups (e.g.,  $R^q$  and  $R^t$  taken together) form an aromatic group, and in another embodiment,  $R^q$  and  $R^t$  taken together form one aromatic group and  $R^r$ , and  $R^p$  taken together form a second aromatic group.

When k is 3 and i is 0, bisphenols containing substituted or 65 unsubstituted cyclohexane units are used, for example bisphenols of formula (8):

HO
$$\begin{array}{c|c}
R^f \\
R^g \\$$

wherein each  $\mathbb{R}^f$  is independently hydrogen,  $C_{1-12}$  alkyl, or halogen; and each  $\mathbb{R}^g$  is independently hydrogen or  $C_{1-12}$  alkyl. The substituents can be aliphatic or aromatic, straight chain, cyclic, bicyclic, branched, saturated, or unsaturated. Such cyclohexane-containing bisphenols, for example the reaction product of two moles of a phenol with one mole of a hydrogenated isophorone, are useful for making polycarbonate polymers with high glass transition temperatures and high heat distortion temperatures. Cyclohexyl bisphenol containing polycarbonates, or a combination comprising at least one of the foregoing with other bisphenol polycarbonates, are supplied by Bayer Co. under the APEC\* trade name.

Other useful dihydroxy compounds having the formula HO—R<sup>1</sup>—OH include aromatic dihydroxy compounds of formula (9):

$$(\mathbb{R}^h)_n$$
 (9)

wherein each  $R^h$  is independently a halogen atom, a  $C_{1-10}$  hydrocarbyl such as a  $C_{1-10}$  alkyl group, a halogen substituted  $C_{1-10}$  hydrocarbyl such as a halogen-substituted  $C_{1-10}$  alkyl group, and n is 0 to 4. The halogen is usually bromine.

Some illustrative examples of dihydroxy compounds include the following: 4,4'-dihydroxybiphenyl, 1,6-dihydroxynaphthalene, 2,6-dihydroxynaphthalene, bis(4-hydroxyphenyl)methane, bis(4-hydroxyphenyl)diphenylmethane, bis(4-hydroxyphenyl)-1-naphthylmethane, 1,2-bis(4-hydroxyphenyl)ethane, 1,1-bis(4-hydroxyphenyl)-1-phenylethane, 2-(4-hydroxyphenyl)-2-(3-hydroxyphenyl)propane, bis(4-hydroxyphenyl)phenylmethane, 2,2-bis(4-hydroxy-3bromophenyl)propane, 1,1-bis (hydroxyphenyl)cyclopentane, 1,1-bis(4-hydroxyphenyl)cyclohexane, 1,1-bis(4-hydroxyphenyl)isobutene, 1,1-bis(4-hydroxyphenyl) cyclododecane, trans-2,3-bis(4-hydroxyphenyl)-2-butene, 2,2-bis(4-hydroxyphenyl)adamantine, alpha,alpha'-bis(4hydroxyphenyetoluene, bis(4-hydroxyphenyl)acetonitrile, 2,2-bis(3-methyl-4-hydroxyphenyl)propane, 2.2-bis(3ethyl-4-hydroxyphenyl)propane, 2,2-bis(3-n-propyl-4-hydroxyphenyl)propane, 2,2-bis(3-isopropyl-4-hydroxyphenyl)propane, 2,2-bis(3-sec-butyl-4-hydroxyphenyl)propane, 2,2-bis(3-t-butyl-4-hydroxyphenyl)propane, 2,2-bis(3-cyclohexyl-4-hydroxyphenyl)propane, 2,2-bis(3-allyl-4-hydroxyphenyl)propane, 2,2-bis(3-methoxy-4-hydroxyphenyl) propane, 2,2-bis(4-hydroxyphenyl)hexafluoropropane, 1,1dichloro-2,2-bis(4-hydroxyphenyl)ethylene, 1,1-dibromo-2, 2-bis(4-hydroxyphenyl)ethylene, 1,1-dichloro-2,2-bis(5phenoxy-4-hydroxyphenyl)ethylene, dihydroxybenzophenone, 3,3-bis(4-hydroxyphenyl)-2-1,6-bis(4-hydroxyphenyl)-1,6-hexanedione, butanone, ethylene glycol bis(4-hydroxyphenyl)ether, bis(4-hydrox-

yphenyl)ether, bis(4-hydroxyphenyl)sulfide, bis(4-hydroxyphenyl)sulfoxide, bis(4-hydroxyphenyl)sulfone, 9,9 to bis (4-hydroxyphenyl)fluorine, 2,7-dihydroxypyrene, 6,6'-dihydroxy-3,3,3',3'-tetramethylspiro(bis)indane

("spirobiindane bisphenol"), 3,3-bis(4-hydroxyphenyl)phthalide, 2,6-dihydroxydibenzo-p-dioxin, 2,6-dihydroxythianthrene, 2,7-dihydroxyphenoxathin, 2,7-dihydroxy-9,10dimethylphenazine, 3,6-dihydroxydibenzofuran, dihydroxydibenzothiophene, and 2,7-dihydroxycarbazole, <sup>10</sup> resorcinol, substituted resorcinol compounds such as 5-methyl resorcinol, 5-ethyl resorcinol, 5-propyl resorcinol, 5-butyl resorcinol, 5-t-butyl resorcinol, 5-phenyl resorcinol, 5-cumyl resorcinol, 2,4,5,6-tetrafluoro resorcinol, 2,4,5,6- 15 tetrabromo resorcinol, or the like; catechol; hydroquinone; substituted hydroquinones such as 2-methyl hydroquinone, 2-ethyl hydroquinone, 2-propyl hydroquinone, 2-butyl hydroquinone, 2-t-butyl hydroquinone, 2-phenyl hydroquinone, 2-cumyl hydroguinone, 2,3,5,6-tetramethyl hydroguinone, 2,3,5,6-tetra-t-butyl hydroquinone, 2,3,5,6-tetrafluoro hydroquinone, 2,3,5,6-tetrabromo hydroquinone, and the like, as well as combinations comprising at least one of the foregoing dihydroxy compounds.

Specific examples of bisphenol compounds that can be represented by formula (3) include 1,1-bis(4-hydroxyphenyl) methane, 1,1-bis(4-hydroxyphenyl)ethane, 2,2-bis(4-hydroxyphenyl)propane (hereinafter "bisphenol-A" or "BPA"), 2,2-bis(4-hydroxyphenyl)butane, 2,2-bis(4-hydroxyphenyl) octane, 1,1-bis(4-hydroxyphenyl)propane, 1,1-bis(4-hydroxyphenyl)propane, 1,1-bis(4-hydroxy-t-butylphenyl)propane, 3,3-bis(4-hydroxyphenyl)phthalimidine, 2-phenyl-3,3-bis(4-hydroxyphenyl)phthalimidine (PPPBP), and 1,1-bis(4-hydroxy-3-methylphenyl)cyclohexane (DMBPC). Combinations comprising at least one of the foregoing dihydroxy compounds can also be used.

"Polycarbonate" as used herein includes homopolycarbonates, copolymers comprising different R¹ moieties in the carbonate (referred to herein as "copolycarbonates"), and copolymers comprising carbonate units and other types of polymer units, such as ester units. In one specific embodiment, the polycarbonate is a linear homopolymer or copolymer comprising units derived from bisphenol-A, in which each of A¹ and A² is p-phenylene and Y¹ is isopropylidene in formula (3). More specifically, at least 60%, particularly at least 80% of the R¹ groups in the polycarbonate are derived from bisphenol-A.

Another specific type of copolymer is a polyester carbonate, also known as a polyester-polycarbonate. Such copolymers further contain, in addition to recurring carbonate chain units of the formula (1), repeating units of formula (10):

wherein D is a divalent group derived from a dihydroxy compound, and can be, for example, a  $C_{2-10}$  alkylene group, a  $C_{6-20}$  alicyclic group, a  $C_{6-20}$  aromatic group or a polyoxy- 65 alkylene group in which the alkylene groups contain 2 to 6 carbon atoms, specifically 2, 3, or 4 carbon atoms; and T

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divalent group derived from a dicarboxylic acid, and can be, for example, a  $C_{2\text{-}10}$  alkylene group, a  $C_{6\text{-}20}$  alicyclic group, a  $C_{6\text{-}20}$  alkyl aromatic group, or a  $C_{6\text{-}20}$  aromatic group.

In one embodiment, D is a C<sub>2-30</sub> alkylene group having a straight chain, branched chain, or cyclic (including polycyclic) structure. In another embodiment, D is derived from an aromatic dihydroxy compound of formula (4) above. In another embodiment, D is derived from an aromatic dihydroxy compound of formula (9) above.

Examples of aromatic dicarboxylic acids that can be used to prepare the polyester units include isophthalic or terephthalic acid, 1,2-di(p-carboxyphenyl)ethane, 4,4'-dicarboxydiphenyl ether, 4,4'-bisbenzoic acid, and combinations comprising at least one of the foregoing acids. Acids containing fused rings can also be present, such as in 1,4-, 1,5-, or 2,6-naphthalenedicarboxylic acids. Specific dicarboxylic acids are terephthalic acid, isophthalic acid, naphthalene dicarboxylic acid, cyclohexane dicarboxylic acid, or combinations thereof. A specific dicarboxylic acid comprises a combination of isophthalic acid and terephthalic acid wherein the weight ratio of isophthalic acid to terephthalic acid is 91:9 to 2:98. In another specific embodiment, D is a  $C_{2-6}$  alkylene group and T is p-phenylene, m-phenylene, naphthalene, a divalent cycloaliphatic group, or a combination thereof. This class of polyester includes the poly(alkylene terephthalates).

The molar ratio of ester units to carbonate units in the copolymers can vary broadly, for example 1:99 to 99:1, specifically 10:90 to 90:10, more specifically 25:75 to 75:25, depending on the desired properties of the final composition.

In a specific embodiment, the polyester unit of a polyester-polycarbonate can be derived from the reaction of a combination of isophthalic and terephthalic diacids (or derivatives thereof) with resorcinol. In another specific embodiment, the polyester unit of a polyester-polycarbonate is derived from the reaction of a combination of isophthalic acid and terephthalic acid with bisphenol-A. In a specific embodiment, the polycarbonate units are derived from bisphenol-A. In another specific embodiment, the polycarbonate units are derived from resorcinol and bisphenol-A in a molar ratio of resorcinol carbonate units to bisphenol-A carbonate units of 1:99 to 90-1

A specific example of a polycarbonate-polyester is a copolycarbonate-polyester-polysiloxane terpolymer comprising carbonate units of formula (1), ester units of formula (10), and polysiloxane (also referred to herein as "polydiorganosiloxane") units of formula (11):

$$\begin{array}{c|c}
R \\
\downarrow \\
SiO \\
\downarrow \\
R
\end{array}$$
(11)

wherein each occurrence of R is same or different, and is a C $_{1-13}$  monovalent organic group. For example, R may independently be a C $_{1-13}$  alkyl group, C $_{1-13}$  alkoxy group, C $_{2-13}$  alkenyl group, C $_{2-13}$  alkenyl group, C $_{3-6}$  cycloalkyl group, C $_{3-6}$  cycloalkoxy group, C $_{6-14}$  aryl group, C $_{6-10}$  aryloxy group, C $_{7-13}$  arylalkyl group, C $_{7-13}$  arylalkoxy group, C $_{7-13}$  alkylaryl group, or C $_{7-13}$  alkylaryloxy group. The foregoing groups may be fully or partially halogenated with fluorine,

chlorine, bromine, or iodine, or a combination thereof. Combinations of the foregoing R groups may be used in the same copolymer. In an embodiment, the polysiloxane comprises R groups that have a minimum hydrocarbon content. In a specific embodiment, an R group with a minimum hydrocarbon content is a methyl group.

The value of E in formula (11) may vary widely depending on the type and relative amount of each component in the thermoplastic composition, the desired properties of the composition, and like considerations. Herein, E can have an average value of 4 to 50. In an embodiment, E has an average value

or, where Ar is derived from bisphenol-A, from dihydroxy aromatic compounds of formula (14):

of 16 to 50, specifically 20 to 45, and more specifically 25 to 45. In another embodiment, E has an average value of 4 to 15, specifically 5 to 15, more specifically 6 to 15, and still more specifically 7 to 12.

In an embodiment, polydiorganosiloxane units are derived from dihydroxy aromatic compound of formula (12):

$$HO \longrightarrow Ar \longrightarrow O \longrightarrow \begin{bmatrix} R \\ | \\ SiO \\ | \\ R \end{bmatrix}_E Ar \longrightarrow OH$$
(12)

wherein E is as defined above; each R may independently be the same or different, and is as defined above; and each Ar may independently be the same or different, and is a substituted or unsubstituted C<sub>6-30</sub> arylene group, wherein the bonds are directly connected to an aromatic moiety. Exemplary Ar groups in formula (12) may be derived from a C<sub>6-30</sub> dihydroxy aromatic compound, for example a dihydroxy aromatic compound of formula (3), (4), (8), or (9) above. Combina- 45 tions comprising at least one of the foregoing dihydroxy aromatic compounds may also be used. Exemplary dihydroxy aromatic compounds are resorcinol (i.e., 1,3-dihydroxybenzene), 4-methyl-1,3-dihydroxybenzene, 5-methyl-1,3-dihydroxybenzene, 4,6-dimethyl-1,3-dihydroxybenzene, 1,4-di-50 hydroxybenzene, 1,1-bis(4-hydroxyphenyl)methane, 1,1-bis (4-hydroxyphenyl)ethane, 2,2-bis(4-hydroxyphenyl) propane, 2,2-bis(4-hydroxyphenyl)butane, 2,2-bis(4hydroxyphenyl)octane, 1,1-bis(4-hydroxyphenyl)propane, 1,1-bis(4-hydroxyphenyl)n-butane, 2,2-bis(4-hydroxy-1methylphenyl)propane, 1,1-bis(4-hydroxyphenyl)cyclohexane, bis(4-hydroxyphenyl sulfide), and 1,1-bis(4-hydroxy-tbutylphenyl)propane. Combinations comprising at least one of the foregoing dihydroxy compounds may also be used. In an embodiment, the dihydroxy aromatic compound is unsubstituted, or is not substituted with non-aromatic hydrocarboncontaining substituents such as, for example, alkyl, alkoxy, or alkylene substituents.

In a specific embodiment, where Ar is derived from resor- 65 cinol, the polydiorganosiloxane repeating units are derived from dihydroxy aromatic compounds of formula (13):

wherein E is as defined above.

In another embodiment, polydiorganosiloxane units are derived from dihydroxy aromatic compound of formula (15):

(15) 
$$HO - R^2 = \begin{bmatrix} R \\ I \\ SIO \end{bmatrix} - \begin{bmatrix} R \\ I \\ R \end{bmatrix} - R^2 - OH$$

wherein R and E are as described above, and each occurrence of  $R^2$  is independently a divalent  $C_{1\text{-}30}$  alkylene or  $C_{7\text{-}30}$  arylene-alkylene, and wherein the polymerized polysiloxane unit is the reaction residue of its corresponding dihydroxy aromatic compound. In a specific embodiment, where  $R^2$  is  $C_{7\text{-}30}$  arylene-alkylene, the polydiorganosiloxane units are derived from dihydroxy aromatic compound of formula (16):

HO 
$$R^3$$
  $R^3$   $R^3$   $R^3$   $R^3$   $R^3$   $R^3$   $R^3$ 

wherein R and E are as defined above. Each  $R^3$  is independently a divalent  $C_{2-8}$  aliphatic group. Each M may be the same or different, and may be a halogen, cyano, nitro,  $C_{1-8}$  alkylthio,  $C_{1-8}$  alkyl,  $C_{1-8}$  alkoxy,  $C_{2-8}$  alkenyl,  $C_{2-8}$  alkenyloxy group,  $C_{3-8}$  cycloalkyl,  $C_{3-8}$  cycloalkoxy,  $C_{6-10}$  aryl,  $C_{6-10}$  aryloxy,  $C_{7-12}$  arylalkyl,  $C_{7-12}$  arylalkoxy,  $C_{7-12}$  alkylaryl, or  $C_{7-12}$  alkylaryloxy, wherein each n is independently 0, 1, 2, 3, or 4.

In an embodiment, M is bromo or chloro, an alkyl group such as methyl, ethyl, or propyl, an alkoxy group such as methoxy, ethoxy, or propoxy, or an aryl group such as phenyl, chlorophenyl, or tolyl;  $R^3$  is a dimethylene, trimethylene or tetramethylene group; and R is a  $C_{1-8}$  alkyl, haloalkyl such as trifluoropropyl, cyanoalkyl, or aryl such as phenyl, chlorophenyl or tolyl. In another embodiment, R is methyl, or a combination of methyl and trifluoropropyl, or a combination

12 bisacetoxypolydiorangonosiloxane and a dihydroxy aro-

of methyl and phenyl. In still another embodiment, M is methoxy, n is 0 or 1,  $R^3$  is a divalent  $C_{1-3}$  aliphatic group, and R is methyl.

In a specific embodiment, the polydiorganosiloxane units are derived from a dihydroxy aromatic compound of formula 5 (17):

$$\begin{array}{c} \text{CH}_{3}\text{O} \\ \text{CH}_{3}\text{O} \\ \end{array} \begin{array}{c} \text{CH}_{3} \\ \text{Si} - \text{O} \\ \text{CH}_{3} \\ \end{array} \begin{array}{c} \text{CH}_{3} \\ \text{Si} \\ \text{CH}_{3} \\ \end{array} \begin{array}{c} \text{CH}_{3} \\ \text{Si} \\ \text{CH}_{3} \\ \end{array} \begin{array}{c} \text{OCH}_{3} \\ \text{OH} \\ \end{array}$$

wherein E is as described above.

In another specific embodiment, the polydiorganosiloxane units are derived from dihydroxy aromatic compound of formula (18):

$$\begin{array}{c|c} & & & \text{CH}_3 \\ \hline & & & \\ \text{Si} & \text{O} \\ \hline & & & \\ \text{CH}_3 \\ \hline & & & \\ \text{CH}_3 \\ \hline & & \\ \text{E-1} \\ \end{array} \begin{array}{c} \text{CH}_3 \\ \hline & \text{OH} \\ \hline \\ \text{CH}_3 \\ \hline \end{array}$$

wherein E is as defined above.

Dihydroxy polysiloxanes typically can be made by func- 35 tionalizing a substituted siloxane oligomer of formula (19):

$$Z = \begin{bmatrix} R \\ I \\ SiO \end{bmatrix} = \begin{bmatrix} R \\ I \\ Si \end{bmatrix} = Z$$

$$\begin{bmatrix} R \\ I \\ R \end{bmatrix}$$

$$\begin{bmatrix} R \\ I \\ I \end{bmatrix}$$

$$\begin{bmatrix} R \\ I \end{bmatrix}$$

$$\begin{bmatrix}$$

wherein R and E are as previously defined, and Z is H, halogen (e.g., Cl, Br, I), or carboxylate. Exemplary carboxylates include acetate, formate, benzoate, and the like. In an exemplary embodiment, where Z is H, compounds of formula (19) may be prepared by platinum catalyzed addition with an aliphatically unsaturated monohydric phenol. Exemplary aliphatically unsaturated monohydric phenols included, for example, eugenol, 2-allylphenol, 4-allylphenol, 4-allyl-2methylphenol, 4-allyl-2-phenylphenol, 4-allyl-2-bromophe-55 nol, 4-allyl-2-t-butoxyphenol, 4-phenyl-2-allylphenol, 2-methyl-4-propenylphenol, 2-allyl-4,6-dimethylphenol, 2-allyl-4-bromo-6-methylphenol, 2-allyl-6-methoxy-4-2-allyl-4,6-dimethylphenol. methylphenol, and Combinations comprising at least one of the foregoing may also be used. Where Z is halogen or carboxylate, functionalization may be accomplished by reaction with a dihydroxy aromatic compound of formulas (3), (4), (8), (9), or a combination comprising at least one of the foregoing dihydroxy 65 aromatic compounds. In an exemplary embodiment, compounds of formula (12) may be formed from an alpha, omega-

matic compound under phase transfer conditions.

Specific copolycarbonate terpolymers include those with polycarbonate units of formula (1) wherein  $R^1$  is a  $C_{6-30}$ arylene group, polysiloxane units derived from siloxane diols of formula (14), (17) or (18), and polyester units wherein T is a C<sub>6-30</sub> arylene group. In an embodiment, T is derived from isophthalic and/or terephthalic acid, or reactive chemical equivalents thereof. In another embodiment, R<sup>1</sup> is derived from the carbonate reaction product of a resorcinol of formula (9), or a combination of a resorcinol of formula (9) and a bisphenol of formula (4).

The relative amount of each type of unit in the foregoing terpolymer will depend on the desired properties of the terpolymer, and are readily determined by one of ordinary skill in the art without undue experimentation, using the guidelines provided herein. For example, the polycarbonate-polyesterpolysiloxane terpolymer can comprise siloxane units in an amount of 0.1 to 25 weight percent (wt %), specifically 0.2 to 10 wt %, more specifically 0.2 to 6 wt %, even more specifically 0.2 to 5 wt %, and still more specifically 0.25 to 2 wt %, based on the total weight of the polycarbonate-polyesterpolysiloxane terpolymer, with the proviso that the siloxane units are provided by polysiloxane units covalently bonded in the polymer backbone of the polycarbonate-polyester-polysiloxane terpolymer. The polycarbonate-polyester-polysiloxane terpolymer can further comprise 0.1 to 49.85 wt % carbonate units, 50 to 99.7 wt % ester units, and 0.2 to 6 wt % polysiloxane units, based on the total weight of the polysiloxane units, ester units, and carbonate units. Alternatively, the polycarbonate-polyester-polysiloxane terpolymer comprises 0.25 to 2 wt % polysiloxane units, 60 to 96.75 wt % ester units, and 3.25 to 39.75 wt % carbonate units, based on the total weight of the polysiloxane units, ester units, and carbonate units.

Various types of thermoplastic compositions are encompassed by embodiments encompassed by this disclosure.

In one embodiment, the polycarbonate can be at least one of the following: a homopolycarbonate derived from a bisphenol; a copolycarbonate derived from more than one bisphenol; and a copolymer derived from one or more bisphenols and having one or more aliphatic ester units or aromatic ester units or siloxane units.

In another embodiment, in addition to the endcapped polycarbonates described above, the thermoplastic compositions can also comprise other thermoplastic polymers, for example polyesters, polyamides, and other polycarbonate homopolymers and copolymers, including polycarbonate-polysiloxane copolymers and polyester carbonates, also known as a polyester-polycarbonates, and polyesters. The polymer component of such compositions can comprise 1 to 99 wt %, specifically 10 to 90, more specifically 20 to 80 wt % of the cyanophenyl endcapped polycarbonate, with the remainder of the polymer component being other polymers.

In another embodiment, a second polycarbonate is formulated with the composition, wherein a second polycarbonate comprises a repeating structure of

$$R^1-O$$

wherein said second polycarbonate is different from said polycarbonate and wherein at least 60 percent of the total number of R<sup>1</sup> groups contain aromatic organic groups and the balance thereof are aliphatic, alicyclic, or aromatic groups.

In another embodiment, the second polycarbonate is derived from bisphenol-A.

The polycarbonates according to embodiments can contain branched polycarbonate(s). Various types of branching agents can be utilized for embodiments encompassed by this 10 disclosure.

Branched polycarbonate blocks can be prepared by adding a branching agent during polymerization. These branching agents include polyfunctional organic compounds containing 15 at least three functional groups selected from hydroxyl, carboxyl, carboxylic anhydride, haloformyl, and mixtures of the foregoing functional groups. Specific examples include trimellitic acid, trimellitic anhydride, trimellitic trichloride (TMTC), tris-p-hydroxy phenyl ethane (THPE), 3,3-bis-(4hydroxyphenyl)-oxindole (also known as isatin-bis-phenol), tris-phenol TC (1,3,5-tris((p-hydroxyphenyl)isopropyl)benzene), tris-phenol PA (4(4(1,1-bis(p-hydroxyphenyl)-ethyl) alpha.alpha-dimethyl benzyl)phenol), 4-chloroformyl 25 phthalic anhydride, trimesic acid, and benzophenone tetracarboxylic acid. The branching agents can be added at a level of 0.05 to 2.0 wt %. Mixtures comprising linear polycarbonates and branched polycarbonates can be used.

In some embodiments, a particular type of branching agent is used to create branched polycarbonate materials. These branched polycarbonate materials have statistically more than two end groups. The branching agent is added in an amount (relative to the bisphenol monomer) that is sufficient to achieve the desired branching content, that is, more than two end groups. The molecular weight of the polymer may become very high upon addition of the branching agent and may lead to viscosity problems during phosgenation. Therefore, in some embodiments, an increase in the amount of the chain termination agent is used in the polymerization. The amount of chain termination agent used when the particular branching agent is used is generally higher than if only a chain termination agent alone is used. The amount of chain termination agent used is generally above 5 mole percent and less than 20 mole percent compared to the bisphenol monomer.

In some embodiments, the branching agent is a structure derived from a triacid trichloride of the formula (21)

$$(Z)_z$$
 $CI$ 
 $CI$ 
 $CI$ 

wherein Z is hydrogen, a halogen,  $C_{1-3}$  alkyl group,  $C_{1-3}$  alkoxy group,  $C_{7-12}$  arylalkyl, alkylaryl, or nitro group, and z 65 is 0 to 3; or a branching agent derived from a reaction with a tri-substituted phenol of the formula (22)

HO 
$$(S)_s$$
  $(S)_s$   $($ 

wherein T is a  $C_{1-20}$  alkyl group,  $C_{1-20}$  alkyleneoxy group,  $C_{7-12}$  arylalkyl, or alkylaryl group, S is hydrogen, a halogen,  $C_{1-3}$  alkyl group,  $C_{1-3}$  alkoxy group,  $C_{7-12}$  arylalkyl, alkylaryl, or nitro group, s is 0 to 4.

In another embodiment, the branching agent is a structure having formula (23)

Examples of specific branching agents that are particularly effective in embodiments include trimellitic trichloride (TMTC), tris-p-hydroxy phenyl ethane (THPE) and isatin-bis-phenol. In one embodiment, in formula (21), Z is hydrogen and z is 3. In another embodiment, in formula (22), S is hydrogen, T is methyl and s is 4.

The relative amount of branching agents used in the manufacture of a polymer according to embodiments will depend on a number of considerations, for example the type of R<sup>1</sup> groups, the amount of cyanophenol, and the desired molecular weight of the polycarbonate. In general, the amount of branching agent is effective to provide about 0.1 to 10 branching units per 100 R<sup>1</sup> units, specifically about 0.5 to 8 branching units per 100 R<sup>1</sup> units, and more specifically about 0.75 to 5 branching units per 100 R<sup>1</sup> units. For branching agents 50 having formula (21), the amount of branching agent tri-ester groups are present in an amount of about 0.1 to 10 branching units per 100 R<sup>1</sup> units, specifically about 0.5 to 8 branching units per 100 R<sup>1</sup> units, and more specifically about 0.75 to 5 tri-ester units per 100 R<sup>1</sup> units. For branching agents having 55 formula (22), the amount of branching agent tricarbonate groups are present in an amount of about 0.1 to 10 branching units per 100 R<sup>1</sup> units, specifically about 0.5 to 8 branching units per 100 R<sup>1</sup> units, and more specifically about 0.75 to 5 tri-phenylcarbonate units per 100 R<sup>1</sup> units. In some embodiments, a combination of two or more branching agents may

In one embodiment, the polycarbonate of a composition has a branching level of greater than or equal to about 1%, or greater than or equal to about 2%, or greater than or equal to about 3%, or about 1% to about 3%.

Various types of end-capping agents can be utilized for embodiments encompassed by this disclosure. In one embodiment, the end-capping agent is selected based upon the molecular weight of said polycarbonate and said branching level imparted by said branching agent.

In another embodiment, the end-capping agents are selected from at least one of the following: phenol or a phenol containing one or more substitutions with at least one of the following: aliphatic groups, olefinic groups, aromatic groups, halogens, ester groups, and ether groups.

In another embodiment, the end-capping agents are selected from at least one of the following: phenol, para-t-butylphenol or para-cumylphenol.

Various types of additives, such as flame retardants, can be utilized in embodiments encompassed herein.

In one embodiment, the flame retardant additives include, for example, flame retardant salts such as alkali metal salts of perfluorinated C<sub>1-16</sub> alkyl sulfonates such as potassium perfluorobutane sulfonate (Rimar salt), potassium perfluoroctane sulfonate, tetraethylammonium perfluorohexane sulfonate, potassium diphenylsulfone sulfonate (KSS), and the 20 like; and salts formed by reacting for example an alkali metal or alkaline earth metal (for example lithium, sodium, potassium, magnesium, calcium and barium salts) and an inorganic acid complex salt, for example, an oxo-anion, such as alkali metal and alkaline-earth metal salts of carbonic acid, such as 25 Na2CO3, K2CO3, MgCO3, CaCO3, and BaCO3 or fluoroanion complex such as Li<sub>3</sub>AlF<sub>6</sub>, BaSiF<sub>6</sub>, KBF<sub>4</sub>, K<sub>3</sub>AlF<sub>6</sub>, KAlF<sub>4</sub>, K<sub>2</sub>SiF<sub>6</sub>, and/or Na<sub>3</sub>AlF<sub>6</sub> or the like. Rimar salt and KSS, alone or in combination with other flame retardants, are particularly useful in the polycarbonate compositions disclosed herein.

In another embodiment, the flame-retardants are selected from at least one of the following: alkali metal salts of perfluorinated  $C_{1-16}$  alkyl sulfonates; potassium perfluorobutane sulfonate; potassium perfluoroctane sulfonate; tetraethylammonium perfluorohexane sulfonate; and potassium diphenyl-sulfone sulfonate.

In another embodiment, the flame retardant is not a bromine or chlorine containing composition.

In another embodiment, the flame retardant additives include organic compounds that include phosphorus, bromine, and/or chlorine. Non-brominated and non-chlorinated phosphorus-containing flame retardants can be used in certain applications for regulatory reasons, for example organic 45 phosphates and organic compounds containing phosphorusnitrogen bonds. One type of exemplary organic phosphate is an aromatic phosphate of the formula (GO)<sub>3</sub>P=O, wherein each G is independently an alkyl, cycloalkyl, aryl, alkylaryl, or arylalkyl group, provided that at least one G is an aromatic 50 group. Two of the G groups can be joined together to provide a cyclic group, for example, diphenyl pentaerythritol diphosphate. Exemplary aromatic phosphates include, phenyl bis (dodecyl)phosphate, phenyl bis(neopentyl)phosphate, phenyl bis(3,5,5'-trimethylhexyl)phosphate, ethyl diphenyl 55 phosphate, 2-ethylhexyl di(p-tolyl)phosphate, bis(2-ethylhexyl)p-tolyl phosphate, tritolyl phosphate, bis(2-ethylhexyl)phenyl phosphate, tri(nonylphenyl)phosphate, bis (dodecyl)p-tolyl phosphate, dibutyl phenyl phosphate, 2-chloroethyl diphenyl phosphate, p-tolyl bis(2,5,5'-trimethylhexyl)phosphate, 2-ethylhexyl diphenyl phosphate, or the like. A specific aromatic phosphate is one in which each G is aromatic, for example, triphenyl phosphate, tricresyl phosphate, isopropylated triphenyl phosphate, and the like.

Di- or poly-functional aromatic phosphorus-containing 65 compounds are also useful, for example, compounds of the formulas below:

$$G^{1}O \xrightarrow{P} G^{2}$$

$$G^{1}O \xrightarrow{P} G^{2}$$

$$G^{2} \xrightarrow{Q} X_{m}$$

$$G^{2} \xrightarrow{Q} G^{2}$$

wherein each G<sup>1</sup> is independently a hydrocarbon having 1 to 30 carbon atoms; each G<sup>2</sup> is independently a hydrocarbon or hydrocarbonoxy having 1 to 30 carbon atoms; each X is independently a bromine or chlorine; m is 0 to 4, and n is 1 to 30. Exemplary di- or polyfunctional aromatic phosphorus-containing compounds include resorcinol tetraphenyl diphosphate (RDP), the bis(diphenyl)phosphate of hydroquinone and the bis(diphenyl)phosphate of bisphenol-A, respectively, their oligomeric and polymeric counterparts, and the like.

Exemplary flame retardant additives containing phosphorus-nitrogen bonds include phosphonitrilic chloride, phosphorus ester amides, phosphoric acid amides, phosphonic acid amides, tris(aziridinyl)phosphine oxide.

Halogenated organic flame retardant compounds can also be used as flame retardants, for example halogenated flame retardant compounds of formula (20):

$$\begin{pmatrix} (\mathbf{Y})_d \\ \mathbf{A} \\ \mathbf$$

wherein R is a  $C_{1-36}$  alkylene, alkylidene or cycloaliphatic linkage, e.g., methylene, ethylene, propylene, isopropylene, isopropylidene, butylene, isobutylene, amylene, cyclohexylene, cyclopentylidene, or the like; or an oxygen ether, carbonyl, amine, or a sulfur-containing linkage, e.g., sulfide, sulfoxide, sulfoxide, or the like. R can also consist of two or more alkylene or alkylidene linkages connected by such groups as aromatic, amino, ether, carbonyl, sulfide, sulfoxide, sulfone, or the like.

Ar and Ar' in formula (20) are each independently mono- or polycarbocyclic aromatic groups such as phenylene, biphenylene, terphenylene, naphthylene, or the like

Y is an organic, inorganic, or organometallic radical, for example (1) halogen, e.g., chlorine, bromine, iodine, fluorine or (2) ether groups of the general formula OB, wherein B is a monovalent hydrocarbon group similar to X or (3) monovalent hydrocarbon groups of the type represented by R or (4) other substituents, e.g., nitro, cyano, and the like, said sub-

stituents being essentially inert provided that there is greater than or equal to one, specifically greater than or equal to two, halogen atoms per aryl nucleus.

When present, each X is independently a monovalent hydrocarbon group, for example an alkyl group such as methyl, ethyl, propyl, isopropyl, butyl, decyl, or the like; an aryl groups such as phenyl, naphthyl, biphenyl, xylyl, tolyl, or the like; and aralkyl group such as benzyl, ethylphenyl, or the like; a cycloaliphatic group such as cyclopentyl, cyclohexyl, or the like. The monovalent hydrocarbon group can itself 10 contain inert substituents.

Each d is independently 1 to a maximum equivalent to the number of replaceable hydrogens substituted on the aromatic rings comprising Ar or Ar'. Each e is independently 0 to a maximum equivalent to the number of replaceable hydrogens on R. Each a, b, and c is independently a whole number, including 0. When b is not 0, neither a nor c can be 0. Otherwise either a or c, but not both, can be 0. Where b is 0, the aromatic groups are joined by a direct carbon-carbon

The hydroxyl and Y substituents on the aromatic groups, Ar and Ar' can be varied in the ortho, meta or para positions on the aromatic rings and the groups can be in any possible geometric relationship with respect to one another.

Included within the scope of the above formula are bisphe- 25 nols of which the following are representative: 2,2-bis-(3,5dichlorophenyl)-propane; bis-(2-chlorophenyl)-methane; bis 1,1-bis-(4-iodophenyl)-(2,6-dibromophenyl)-methane; ethane; 1,2-bis-(2,6-dichlorophenyl)-ethane; 1,1-bis-(2chloro-4-iodophenyl)ethane; 1,1-bis-(2-chloro-4- 30 methylphenyl)-ethane; 1,1-bis-(3,5-dichlorophenyl)-ethane; 2,2-bis-(3-phenyl-4-bromophenyl)-ethane; 2,6-bis-(4,6dichloronaphthyl)-propane; 2,2-bis-(2,6-dichlorophenyl)pentane; 2,2-bis-(3,5-dibromophenyl)-hexane; bis-(4-chlorophenyl)-phenyl-methane; bis-(3,5-dichlorophenyl)- 35 cyclohexylmethane; bis-(3-nitro-4-bromophenyl)-methane; bis-(4-hydroxy-2,6-dichloro-3-methoxyphenyl)-methane; and 2,2-bis-(3,5-dichloro-4-hydroxyphenyl)-propane 2,2 bis-(3-bromo-4-hydroxyphenyl)-propane. Also included 1,4-dibromobenzene, 1,3-dichloro-4-hydroxybenzene, and biphenyls such as 2,2'-dichlorobiphenyl, polybrominated 1,4-diphenoxybenzene, 2,4'-dibromobiphenyl, and 2,4'dichlorobiphenyl as well as decabromo diphenyl oxide, and the like.

Another useful class of flame retardant is the class of cyclic siloxanes having the general formula (R<sub>2</sub>SiO), wherein R is a monovalent hydrocarbon or fluorinated hydrocarbon having from 1 to 18 carbon atoms and y is a number from 3 to 12. Examples of fluorinated hydrocarbon include, but are not 50 limited to, 3-fluoropropyl, 3,3,3-trifluoropropyl, 5,5,5,4,4,3, 3-heptafluoropentyl, fluorophenyl, difluorophenyl and trifluorotolyl. Examples of exemplary cyclic siloxanes include, but are not limited to, octamethylcyclotetrasiloxane, 1,2,3,4tetramethyl-1,2,3,4-tetravinylcyclotetrasiloxane, 1,2,3,4-tet-55 ramethyl-1,2,3,4-tetraphenylcyclotetrasiloxane, octaethyloctapropylcyclotetrasiloxane, cyclotetrasiloxane, octabutylcyclotetrasiloxane, decamethylcyclopentasiloxane, dodecamethylcyclohexasiloxane, tetradecamethylcycloheptasiloxane, hexadecamethylcyclooctasiloxane, eicosameth- 60 ylcyclodecasiloxane, octaphenylcyclotetrasiloxane, and the like. A particularly useful cyclic siloxane is octaphenylcyclotetrasiloxane.

When present, the foregoing flame retardant additives are generally present in amounts of 0.01 to 10 wt %, more specifically 0.02 to 5 wt %, based on 100 parts by weight of the polymer component of the thermoplastic composition.

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In another embodiment, the thermoplastic composition can further include an impact modifier(s), with the proviso that the additives are selected so as to not significantly adversely affect the desired properties of the thermoplastic composition. Exemplary impact modifiers are typically high molecular weight elastomeric materials derived from olefins, monovinyl aromatic monomers, acrylic and methacrylic acids and their ester derivatives, as well as conjugated dienes. The polymers formed from conjugated dienes can be fully or partially hydrogenated. The elastomeric materials can be in the form of homopolymers or copolymers, including random, block, radial block, graft, and core-shell copolymers. Combinations of impact modifiers can be used.

A specific type of impact modifier is an elastomer-modified graft copolymer comprising (i) an elastomeric (i.e., rubbery) polymer substrate having a glass transition temperature  $(T_{\rho})$  less than  $10^{\circ}$  C., more specifically less than  $-10^{\circ}$  C., or more specifically -40° to -80° C., and (ii) a rigid polymeric superstrate grafted to the elastomeric polymer substrate. Materials for use as the elastomeric phase include, for example, conjugated diene rubbers, for example polybutadiene and polyisoprene; copolymers of a conjugated diene with less than 50 wt % of a copolymerizable monomer, for example a monovinylic compound such as styrene, acrylonitrile, n-butyl acrylate, or ethyl acrylate; olefin rubbers such as ethylene propylene copolymers (EPR) or ethylene-propylene-diene monomer rubbers (EPDM); ethylene-vinyl acetate rubbers; silicone rubbers; elastomeric C<sub>1-8</sub> alkyl(meth)acrylates; elastomeric copolymers of C<sub>1-8</sub> alkyl(meth)acrylates with butadiene and/or styrene; or combinations comprising at least one of the foregoing elastomers. Materials for use as the rigid phase include, for example, monovinyl aromatic monomers such as styrene and alpha-methyl styrene, and monovinylic monomers such as acrylonitrile, acrylic acid, methacrylic acid, and the  $C_1$ - $C_6$  esters of acrylic acid and methacrylic acid, specifically methyl methacrylate. As used herein, the term "(meth)acrylate" encompasses both acrylate and methacrylate groups.

Specific exemplary elastomer-modified graft copolymers within the above structural formula are: 1,3-dichlorobenzene, 40 include those formed from styrene-butadiene-styrene (SBS), styrene-butadiene rubber (SBR), styrene-ethylene-butadiene-styrene (SEBS), ABS (acrylonitrile-butadiene-styrene), acrylonitrile-ethylene-propylene-diene-styrene (AES), styrene-isoprene-styrene (SIS), methyl methacrylate-butadienestyrene (MBS), and styrene-acrylonitrile (SAN).

Impact modifiers, when present, are generally present in amounts of 1 to 30 wt %, based on 100 parts by weight of the polymer component of the thermoplastic composition.

According to an embodiment, the thermoplastic composition also can include various additives ordinarily incorporated in polycarbonate compositions of this type, with the proviso that the additives are selected so as to not significantly adversely affect the desired properties of the polycarbonate, for example, transparency and flame retardance. Combinations of additives can be used. Such additives can be mixed at a suitable time during the mixing of the components for forming the composition.

Various additives can be incorporated into the composition of matters encompassed by embodiments disclosed herein.

In one embodiment, one or more additives are selected from at least one of the following: UV stabilizing additives, thermal stabilizing additives, mold release agents, colorants, organic and inorganic fillers, and gamma-stabilizing agents.

Possible fillers or reinforcing agents include, for example, silicates and silica powders such as aluminum silicate (mullite), synthetic calcium silicate, zirconium silicate, fused silica, crystalline silica graphite, natural silica sand, or the

like; boron powders such as boron-nitride powder, boronsilicate powders, or the like; oxides such as TiO<sub>2</sub>, aluminum oxide, magnesium oxide, or the like; calcium sulfate (as its anhydride, dihydrate or trihydrate); calcium carbonates such as chalk, limestone, marble, synthetic precipitated calcium 5 carbonates, or the like; talc, including fibrous, modular, needle shaped, lamellar talc, or the like; wollastonite; surfacetreated wollastonite; glass spheres such as hollow and solid glass spheres, silicate spheres, cenospheres, aluminosilicate (armospheres), or the like; kaolin, including hard kaolin, soft kaolin, calcined kaolin, kaolin comprising various coatings known in the art to facilitate compatibility with the polycarbonate polymeric matrix, or the like; single crystal fibers or "whiskers" such as silicon carbide, alumina, boron carbide, iron, nickel, copper, or the like; fibers (including continuous and chopped fibers) such as asbestos, carbon fibers, glass fibers, such as E, A, C, ECR, R, S, D, or NE glasses, or the like; sulfides such as molybdenum sulfide, zinc sulfide or the like; barium compounds such as barium titanate, barium ferrite, barium sulfate, heavy spar, or the like; metals and metal 20 oxides such as particulate or fibrous aluminum, bronze, zinc, copper and nickel or the like; flaked fillers such as glass flakes, flaked silicon carbide, aluminum diboride, aluminum flakes, steel flakes or the like; fibrous fillers, for example short inorganic fibers such as those derived from blends comprising 25 at least one of aluminum silicates, aluminum oxides, magnesium oxides, and calcium sulfate hemihydrate or the like; natural fillers and reinforcements, such as wood flour obtained by pulverizing wood, fibrous products such as cellulose, cotton, sisal, jute, starch, cork flour, lignin, ground nut 30 shells, corn, rice grain husks or the like; organic fillers such as polytetrafluoroethylene; reinforcing organic fibrous fillers formed from organic polymers capable of forming fibers such as poly(ether ketone), polyimide, polybenzoxazole, poly (phenylene sulfide), polyesters, polyethylene, aromatic 35 polyamides, aromatic polyimides, polyetherimides, polytetrafluoroethylene, acrylic resins, poly(vinyl alcohol) or the like; as well as additional fillers and reinforcing agents such as mica, clay, feldspar, flue dust, fillite, quartz, quartzite, perlite, tripoli, diatomaceous earth, carbon black, or the like, 40 or combinations comprising at least one of the foregoing fillers or reinforcing agents.

The fillers and reinforcing agents can be coated with a layer of metallic material to facilitate conductivity, or surface treated with silanes to improve adhesion and dispersion with 45 the polycarbonate polymeric matrix. In addition, the reinforcing fillers can be provided in the form of monofilament or multifilament fibers and can be used individually or in combination with other types of fiber, through, for example, coweaving or core/sheath, side-by-side, orange-type or matrix 50 and fibril constructions, or by other methods known to one skilled in the art of fiber manufacture. Exemplary co-woven structures include, for example, glass fiber-carbon fiber, carbon fiber-aromatic polyimide (aramid) fiber, and aromatic polyimide fiberglass fiber or the like. Fibrous fillers can be 55 supplied in the form of, for example, rovings, woven fibrous reinforcements, such as 0-90 degree fabrics or the like; nonwoven fibrous reinforcements such as continuous strand mat, chopped strand mat, tissues, papers and felts or the like; or three-dimensional reinforcements such as braids. Fillers are 60 generally used in amounts of 0 to 80 parts by weight, based on 100 parts by weight of the polymer component of the composition.

Exemplary antioxidant additives include, for example, organophosphites such as tris(nonyl phenyl)phosphite, tris(2, 65 4-di-t-butylphenyl)phosphite (e.g., "IRGAFOS 168" or "I-168"), bis(2,4-di-t-butylphenyl)pentaerythritol diphos-

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phite, distearyl pentaerythritol diphosphite or the like; alkylated monophenols or polyphenols; alkylated reaction products of polyphenols with dienes, such as tetrakis[methylene (3,5-di-tert-butyl-4-hydroxyhydrocinnamate)]methane, the like; butylated reaction products of para-cresol or dicyclopentadiene; alkylated hydroquinones; hydroxylated thiodiphenyl ethers; alkylidene-bisphenols; benzyl compounds; esters of beta-(3,5-di-tert-butyl-4-hydroxyphenyl)-propionic acid with monohydric or polyhydric alcohols; esters of beta-(5-tert-butyl-4-hydroxy-3-methylphenyl)-propionic with monohydric or polyhydric alcohols; esters of thioalkyl or thioaryl compounds such as distearylthiopropionate, dilaurylthiopropionate, ditridecylthiodipropionate, octadecyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate, pentaerythrityl-tetrakis[3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate or the like; amides of beta-(3,5-di-tert-butyl-4-

hydroxyphenyl)-propionic acid or the like, or combinations comprising at least one of the foregoing antioxidants. Antioxidants are generally used in amounts of 0.0001 to 1 part by weight, based on 100 parts by weigh of the polymer component of the thermoplastic composition (excluding any filler).

Exemplary heat stabilizer additives include, for example, organophosphites such as triphenyl phosphite, tris-(2,6-dimethylphenyl)phosphite, tris-(mixed mono- and di-nonylphenyl)phosphite or the like; phosphonates such as dimethylbenzene phosphonate or the like, phosphates such as trimethyl phosphate, or the like, or combinations comprising at least one of the foregoing heat stabilizers. Heat stabilizers are generally used in amounts of 0.0001 to 1 part by weight, based on 100 parts by weight of the polymer component of the thermoplastic composition.

Light stabilizers and/or ultraviolet light (UV) absorbing additives can also be used. Exemplary light stabilizer additives include, for example, benzotriazoles such as 2-(2-hydroxy-5-methylphenyl)benzotriazole, 2-(2-hydroxy-5-tertoctylphenyl)-benzotriazole and 2-hydroxy-4-n-octoxy benzophenone, or the like, or combinations comprising at least one of the foregoing light stabilizers. Light stabilizers are generally used in amounts of 0.0001 to 1 parts by weight, based on 100 parts by weight of the polymer component of the thermoplastic composition, according to embodiments.

Exemplary UV absorbing additives include for example, hydroxybenzophenones; hydroxybenzotriazoles; hydroxybenzotriazines; cyanoacrylates; oxanilides; benzoxazinones; 2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)-phenol (CYASORB® 5411); 2-hydroxy-4-n-octyloxybenzophenone (CYASORB® 531); 2-[4,6-bis(2,4-dimethylphenyl)-1, 3,5-triazin-2-yl]-5-(octyloxy)-phenol (CYASORB® 1164); 2,2'-(1,4-phenylene)bis(4H-3,1-benzoxazin-4-one) (CYA-SORB® UV-3638); 1,3-bis[(2-cyano-3,3-diphenylacryloyl) oxy]-2,2-bis[[(2-cyano-3,3-diphenylacryloyl)oxy]methyl] propane (UVINUL® 3030); 2,2'-(1,4-phenylene)bis(4H-3,1benzoxazin-4-one); 1,3-bis[(2-cyano-3,3-diphenylacryloyl) oxy]-2,2-bis[[(2-cyano-3,3-diphenylacryloyl)oxy]methyl] propane; nano-size inorganic materials such as titanium oxide, cerium oxide, and zinc oxide, all with particle size less than or equal to 100 nanometers; or the like, or combinations comprising at least one of the foregoing UV absorbers. UV absorbers are generally used in amounts of 0.0001 to 1 part by weight, based on 100 parts by weight of the polymer component of the thermoplastic composition.

Plasticizers, lubricants, and/or mold release agents can also be used. There is considerable overlap among these types of materials, which include, for example, phthalic acid esters such as dioctyl-4,5-epoxy-hexahydrophthalate; tris-(octoxy-carbonylethyl)isocyanurate; tristearin; di- or polyfunctional aromatic phosphates such as resorcinol tetraphenyl diphos-

phate (RDP), the bis(diphenyl)phosphate of hydroquinone and the bis(diphenyl)phosphate of bisphenol-A; poly-alphaolefins; epoxidized soybean oil; silicones, including silicone oils; esters, for example, fatty acid esters such as alkyl stearyl esters, e.g., methyl stearate, stearyl stearate, pentaerythritol 5 tetrastearate (PETS), and the like; combinations of methyl stearate and hydrophilic and hydrophobic nonionic surfactants comprising polyethylene glycol polymers, polypropylene glycol polymers, poly(ethylene glycol-co-propylene glycol) copolymers, or a combination comprising at least one of the foregoing glycol polymers, e.g., methyl stearate and polyethylene-polypropylene glycol copolymer in a suitable solvent; waxes such as beeswax, montan wax, paraffin wax, or the like. Such materials are generally used in amounts of 0.001 to 1 part by weight, specifically 0.01 to 0.75 part by 15 weight, more specifically 0.1 to 0.5 part by weight, based on 100 parts by weight of the polymer component of the thermoplastic composition.

The term "antistatic agent" refers to monomeric, oligomeric, or polymeric materials that can be processed into 20 polymer resins and/or sprayed onto materials or articles to improve conductive properties and overall physical performance. Examples of monomeric antistatic agents include glycerol monostearate, glycerol distearate, glycerol tristearate, ethoxylated amines, primary, secondary and tertiary 25 amines, ethoxylated alcohols, alkyl sulfates, alkylarylsulfates, alkylphosphates, alkylaminesulfates, alkyl sulfonate salts such as sodium stearyl sulfonate, sodium dodecylbenzenesulfonate or the like, quaternary ammonium salts, quaternary ammonium resins, imidazoline derivatives, sorbitan 30 esters, ethanolamides, betaines, or the like, or combinations comprising at least one of the foregoing monomeric antistatic agents.

Exemplary polymeric antistatic agents include certain polyesteramides polyether-polyamide (polyetheramide) 35 block copolymers, polyetheresteramide block copolymers, polyetheresters, or polyurethanes, each containing polyalkylene glycol moieties polyalkylene oxide units such as polyethylene glycol, polypropylene glycol, polytetramethylene glycol, and the like. Such polymeric antistatic agents are 40 commercially available, for example PELESTAT\* 6321 (Sanyo) or PEBAX\* MH1657 (Atofina), IRGASTAT\* P18 and P22 (Ciba-Geigy). Other polymeric materials that can be used as antistatic agents are inherently conducting polymers such as polyaniline (commercially available PANIPOL\*EB from Panipol), polypyrrole and polythiophene (commercially available from Bayer), which retain some of their intrinsic conductivity after melt processing at elevated temperatures. In one embodiment, carbon fibers, carbon nanofibers, carbon nanotubes, carbon black, or a com- 50 bination comprising at least one of the foregoing can be used in a polymeric resin containing chemical antistatic agents to render the composition electrostatically dissipative. Antistatic agents are generally used in amounts of 0.0001 to 5 parts by weight, based on 100 parts by weight (pbw) of the 55 polymer component of the thermoplastic composition.

Colorants such as pigment and/or dye additives can also be present provided they do not adversely affect, for example, any flame retardant performance. Useful pigments can include, for example, inorganic pigments such as metal 60 oxides and mixed metal oxides such as zinc oxide, titanium dioxides, iron oxides, or the like; sulfides such as zinc sulfides, or the like; aluminates; sodium sulfo-silicates sulfates, chromates, or the like; carbon blacks; zinc ferrites; ultramarine blue; organic pigments such as azos, di-azos, quinacridones, perylenes, naphthalene tetracarboxylic acids, flavanthrones, isoindolinones, tetrachloroisoindolinones,

anthraquinones, enthrones, dioxazines, phthalocyanines, and azo lakes; Pigment Red 101, Pigment Red 122, Pigment Red 149, Pigment Red 177, Pigment Red 179, Pigment Red 202, Pigment Violet 29, Pigment Blue 15, Pigment Blue 60, Pigment Green 7, Pigment Yellow 119, Pigment Yellow 147, Pigment Yellow 150, and Pigment Brown 24; or combinations comprising at least one of the foregoing pigments. Pigments are generally used in amounts of 0.01 to 10 parts by weight, based on 100 parts by weight of the polymer component of the thermoplastic composition.

Exemplary dyes are generally organic materials and include, for example, coumarin dyes such as coumarin 460 (blue), coumarin 6 (green), nile red or the like; lanthanide complexes; hydrocarbon and substituted hydrocarbon dyes; polycyclic aromatic hydrocarbon dyes; scintillation dyes such as oxazole or oxadiazole dyes; aryl- or heteroaryl-substituted poly(C2-8) olefin dyes; carbocyanine dyes; indanthrone dyes; phthalocyanine dyes; oxazine dyes; carbostyryl dyes; napthalenetetracarboxylic acid dyes; porphyrin dyes; bis(styryl)biphenyl dyes; acridine dyes; anthraquinone dyes; cyanine dyes; methine dyes; arylmethane dyes; azo dyes; indigoid dyes, thioindigoid dyes, diazonium dyes; nitro dyes; quinone imine dyes; aminoketone dyes; tetrazolium dyes; thiazole dyes; perylene dyes, perinone dyes; bis-benzoxazolylthiophene (BBOT); triarylmethane dyes; xanthene dyes; thioxanthene dyes; naphthalimide dyes; lactone dyes; fluorophores such as anti-stokes shift dyes which absorb in the near infrared wavelength and emit in the visible wavelength, or the like; luminescent dyes such as 7-amino-4-methylcoumarin; 3-(2'-benzothiazolyl)-7-diethylaminocou-2-(4-biphenylyl)-5-(4-t-butylphenyl)-1,3,4marin; oxadiazole; 2,5-bis-(4-biphenylyl)-oxazole; 2,2'-dimethyl-pquaterphenyl; 2,2-dimethyl-p-terphenyl; 3,5,3"",5""-tetra-t-2,5-diphenylfuran; butyl-p-quinquephenyl; diphenyloxazole; 4,4'-diphenylstilbene; 4-dicyanomethylene-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran; 1,1'-diethyl-2,2'-carbocyanine iodide; 3,3'-diethyl-4,4',5,5'-dibenzothiatricarbocyanine iodide; 7-dimethylamino-1-methyl-4-methoxy-8-azaquinolone-2; 7-dimethylamino-4-methylquinolone-2; 2-(4-(4-dimethylaminophenyl)-1,3-butadienyl)-3-ethylbenzothiazolium perchlorate; 3-diethylamino-7-diethyliminophenoxazonium perchlorate; 2-(1-naphthyl)-5-phenyloxazole; 2,2'-p-phenylen-bis(5-phenyloxazole); rhodamine 700; rhodamine 800; pyrene, chrysene, rubrene, coronene, or the like; or combinations comprising at least one of the foregoing dyes.

Where a foam is desired, useful blowing agents include, for example, low boiling halohydrocarbons and those that generate carbon dioxide; blowing agents that are solid at room temperature and when heated to temperatures higher than their decomposition temperature, generate gases such as nitrogen, carbon dioxide, and ammonia gas, such as azodicarbonamide, metal salts of azodicarbonamide, 4,4' oxybis (benzenesulfonylhydrazide), sodium bicarbonate, ammonium carbonate, or the like, or combinations comprising at least one of the foregoing blowing agents. Blowing agents are generally used in amounts of 0.01 to 20 parts by weight, based on 100 parts by weight of the polymer component of the thermoplastic composition.

Dyes are generally used in amounts of 0.01 to 10 parts by

weight, based on 100 parts by weight of the polymer compo-

nent of the thermoplastic composition.

Anti-drip agents can also be used in the thermoplastic composition according to embodiments, for example a fibril forming or non-fibril forming fluoropolymer such as polytetrafluoroethylene (PTFE). The anti-drip agent can be encapsulated by a rigid copolymer as described above, for example

styrene-acrylonitrile copolymer (SAN). PTFE encapsulated in SAN is known as TSAN. Encapsulated fluoropolymers can be made by polymerizing the encapsulating polymer in the presence of the fluoropolymer, for example an aqueous dispersion. TSAN can provide significant advantages over 5 PTFE, in that TSAN can be more readily dispersed in the composition. An exemplary TSAN can comprise 50 wt % PTFE and 50 wt % SAN, based on the total weight of the encapsulated fluoropolymer. The SAN can comprise, for example, 75 wt % styrene and 25 wt % acrylonitrile based on 10 the total weight of the copolymer. Alternatively, the fluoropolymer can be pre-blended in some manner with a second polymer, such as for, example, an aromatic polycarbonate or SAN to form an agglomerated material for use as an anti-drip agent. Either method can be used to produce an encapsulated 15 fluoropolymer. Antidrip agents are generally used in amounts of 0.1 to 5 percent by weight, based on 100 parts by weight of the polymer component of the thermoplastic composition.

Radiation stabilizers can also be present, specifically gamma-radiation stabilizers. Exemplary gamma-radiation 20 stabilizers include alkylene polyols such as ethylene glycol, propylene glycol, 1,3-propanediol, 1,2-butanediol, 1,4-butanediol, meso-2,3-butanediol, 1,2-pentanediol, 2,3-pentanediol, 1,4-pentanediol, 1,4-hexandiol, and the like; cycloalkylene polyols such as 1,2-cyclopentanediol, 1,2-cy-25 clohexanediol, and the like; branched alkylenepolyols such as 2,3-dimethyl-2,3-butanediol (pinacol), and the like, as well as alkoxy-substituted cyclic or acyclic alkanes. Unsaturated alkenols are also useful, examples of which include 4-methyl-4penten-2-ol, 3-methyl-pentene-3-ol, 2-methyl-4-penten-2- 30 ol, 2,4-dimethyl-4-pene-2-ol, and 9 to decen-1-ol, as well as tertiary alcohols that have at least one hydroxy substituted tertiary carbon, for example 2-methyl-2,4-pentanediol (hexylene glycol), 2-phenyl-2-butanol, 3-hydroxy-3-methyl-2-butanone, 2-phenyl-2-butanol, and the like, and cyclic tertiary 35 alcohols such as 1-hydroxy-1-methyl-cyclohexane. Certain hydroxymethyl aromatic compounds that have hydroxy substitution on a saturated carbon attached to an unsaturated carbon in an aromatic ring can also be used. The hydroxysubstituted saturated carbon can be a methylol group 40 (—CH<sub>2</sub>OH) or it can be a member of a more complex hydrocarbon group such as —CR<sup>4</sup>HOH or —CR<sup>4</sup>OH wherein R<sup>4</sup> is a complex or a simple hydrocarbon. Specific hydroxy methyl aromatic compounds include benzhydrol, 1,3-benzenedimethanol, benzyl alcohol, 4-benzyloxy benzyl alcohol and 45 benzyl benzyl alcohol. 2-Methyl-2,4-pentanediol, polyethylene glycol, and polypropylene glycol are often used for gamma-radiation stabilization. Gamma-radiation stabilizing compounds are typically used in amounts of 0.1 to 10 parts by weight based on 100 parts by weight of the polymer component of the thermoplastic composition.

Thermoplastic compositions according to embodiments can be manufactured by various methods. For example, the desired constituents such as, for example, polycarbonate, flame retardant, impact modifier (if present), and/or other 55 optional components can be first blended in a HENSCHEL-Mixer\* high speed mixer. Other low shear processes, including but not limited to hand mixing, can also accomplish this blending. The blend is then fed into the throat of a single or twin-screw extruder via a hopper. Alternatively, at least one of 60 the components can be incorporated into the composition by feeding directly into the extruder at the throat and/or downstream through a sidestuffer. Additives can also be compounded into a masterbatch with a desired polymeric resin and fed into the extruder. The extruder is generally operated at 65 a temperature higher than that necessary to cause the composition to flow. The extrudate is immediately quenched in a

water batch and pelletized. The pellets, so prepared, when cutting the extrudate can be one-fourth inch long or less as desired. Such pellets can be used for subsequent molding, shaping, or forming.

In some embodiments described above, the onset of high-temperature cross-linking can be controlled by adjusting the molecular weight of the end-capped polycarbonate or by the addition of certain flame retardant salts, in particular alkali metal salts of perfluorinated  $C_{1\text{--}16}$  alkyl sulfonates. In one embodiment, the addition of an inorganic flame retardant (e.g., KSS) increases the temperature of the onset of cross-linking/branching in the polycarbonate by 20 to 80° C., specifically 40 to 60° C.

Shaped, formed, or molded articles comprising the thermoplastic compositions are also provided, according to embodiments. The thermoplastic compositions can be molded into useful shaped articles by a variety of means such as injection molding, extrusion, rotational molding, blow molding and thermoforming to form articles such as, for example, computer and business machine housings such as housings for monitors, handheld electronic device housings such as housings for cell phones, electrical connectors, and components of lighting fixtures, ornaments, home appliances, roofs, greenhouses, sun rooms, swimming pool enclosures, thin walled articles such as housing for electronic devices and the like. Additional examples of articles that can be formed from the compositions include electrical parts, such as relays, and enclosures, consumer electronics such as enclosures and parts for laptops, desktops, docking stations, personal digital assistants (PDAs), digital cameras, desktops, and telecommunications parts such as parts for base station terminals. Further examples of articles that can be formed from compositions include light guides, light guide panels, lenses, covers, sheets, films, and the like, e.g., LED lenses, LED covers, and so forth.

Interfacial Polymerization

In accordance with embodiments, polycarbonates having enhanced optical qualities can be manufactured by an interfacial polymerization process. Although the reaction conditions for interfacial polymerization can vary, an exemplary process generally involves dissolving or dispersing a dihydric phenol reactant in aqueous caustic soda or potash, adding the resulting mixture to a water-immiscible solvent medium, and contacting the reactants with a carbonate precursor in the presence of a catalyst such as, for example, triethylamine or a phase transfer catalyst, under controlled pH conditions, e.g., 8 to 11. The most commonly used water immiscible solvents include methylene chloride, 1,2-dichloroethane, chlorobenzene, toluene, and the like.

Exemplary carbonate precursors include, for example, a carbonyl halide such as carbonyl bromide or carbonyl chloride, or a haloformate such as a bishaloformates of a dihydric phenol (e.g., the bischloroformates of bisphenol-A, hydroquinone, or the like) or a glycol (e.g., the bishaloformate of ethylene glycol, neopentyl glycol, polyethylene glycol, or the like). Combinations comprising at least one of the foregoing types of carbonate precursors can also be used. In an exemplary embodiment, an interfacial polymerization reaction to form carbonate linkages uses phosgene as a carbonate precursor, and is referred to as a phosgenation reaction.

Among the phase transfer catalysts that can be used are catalysts of the formula  $(R_3)_4Q+X$ , wherein each  $R_3$  is the same or different, and is a  $C_{1-10}$  alkyl group; Q is a nitrogen or phosphorus atom; and X is a halogen atom or a  $C_{1-8}$  alkoxy group or  $C_{6-18}$  aryloxy group. Exemplary phase transfer catalysts include, for example,  $[CH_3(CH_2)_3]_4NX$ ,  $[CH_3(CH_2)_3]_4PX$ ,  $[CH_3(CH_2)_5]_4NX$ ,  $[CH_3(CH_2)_6]_4NX$ ,

 $[\mathrm{CH_3}(\mathrm{CH_2})_4]_4\mathrm{NX},\ \mathrm{CH_3}[\mathrm{CH_3}(\mathrm{CH_2})_3]_3\mathrm{NX},\ \mathrm{and}\ \mathrm{CH_3}[\mathrm{CH_3}(\mathrm{CH_2})_2]_3\mathrm{NX},\ \mathrm{wherein}\ \mathrm{X}\ \mathrm{is}\ \mathrm{Cl--},\mathrm{Br--},\mathrm{a}\ \mathrm{C}_{1\text{--}8}\ \mathrm{alkoxy}\ \mathrm{group}\ \mathrm{or}\ \mathrm{a}\ \mathrm{C}_{6\text{--}18}\ \mathrm{aryloxy}\ \mathrm{group}. \mathrm{An}\ \mathrm{effective}\ \mathrm{amount}\ \mathrm{of}\ \mathrm{a}\ \mathrm{phase}\ \mathrm{transfer}\ \mathrm{catalyst}\ \mathrm{can}\ \mathrm{be}\ 0.1\ \mathrm{to}\ 10\ \mathrm{wt}\ \%\ \mathrm{based}\ \mathrm{on}\ \mathrm{the}\ \mathrm{weight}\ \mathrm{of}\ \mathrm{bisphenol}\ \mathrm{in}\ \mathrm{the}\ \mathrm{phosgenation}\ \mathrm{mixture}.$  In another embodiment, an effective amount of phase transfer catalyst can be  $0.5\ \mathrm{to}\ 2\ \mathrm{wt}\ \%\ \mathrm{based}\ \mathrm{on}\ \mathrm{the}\ \mathrm{weight}\ \mathrm{of}\ \mathrm{bisphenol}\ \mathrm{in}\ \mathrm{the}\ \mathrm{phosgenation}\ \mathrm{mixture}.$ 

In one embodiment, the polycarbonate encompassed by this disclosure is made by an interfacial polymerization process. One of ordinary skill in the art would be able to carry out an interfacial process without undue experimentation.

In another embodiment, the polycarbonate encompassed by this disclosure excludes the utilization of a melt polymerization process to make at least one of said polycarbonates.

Protocols may be adjusted so as to obtain a desired product within the scope of the disclosure and this can be done without undue experimentation. A desired product is in one embodiment to achieve a molded article of the composition having a transmission level higher than 90.0%, as measured 20 by ASTM D1003, at 2.5 mm thickness and a YI lower than 1.5, as measured by ASTM D1925, with an increase in YI lower than 2 during 2000 hours of heat aging at 130° C. made by an interfacial process.

Embodiments are further illustrated by the following non- 25 limiting example/experimentation.

#### **EXAMPLE**

In order to test the effect of process parameters on resin 30 color, all resins were tested in a simple, fixed formulation with only 0.05% tris(di-t-butylphenyl)phosphite. Such a formulation may not give optimal results but allows differences in resin color to be observed. Granulate was molded into 2.5 mm thickness color plaques which were used for color measurements. Transmission was measured on a Gardner Dual Hazeguard according to ASTM D1003 as disclosed above. Yellowness Index (YI) was calculated from the absorption spectrum from a MacBeth 9000A according to ASTM D1925. Heat aging was done by placing color plaques in an oven at 130° C. 40 Color was measured at regular intervals over a period of 5,000 hours (hrs).

It is noted that in addition to the afore-referenced heat stabilizer tris(di-t-butylphenyl)phosphite (Irgafos 168), the inventors have determined that triphenyl phosphine (TPP) 45 and Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate (Ultranxo 1076) also can be effective, according to embodiments.

PC resin was depolymerized by adding 3 ml of tetrahydrofuran and 3 milliliters (ml) of 10% w KOH in methanol to 50 about 200 mg of resin or plastic. After shaking the solution for 60 minutes, the carbonate precipitate was dissolved by adding 3 ml glacial acetic acid. The resulting mixture was analyzed using a method similar to the one described by J. Poskrobko et al., Journal of Chromatography A., 883, 291-297 (2000), 55 which is herein incorporated by reference. Note that the results are essentially the sum of any residual, unreacted monomer and impurities that are in the plastic and those that have reacted and have been incorporated in the chain.

BPX-1 was synthesized according to a procedure by 60 Nowakowska et al., Polish J. Appl. Chem. X1(3), 247-254 (1996) and 9,9' Dimethyxanthene (DMX) 96% was purchased from Sigma-Aldrich and used without any further purification.

4-(4'-hydroxyphenyl)2,2,4-trimethylchroman (chroman), 65 was prepared from the melted mixture of mesityl oxide and phenol. The mixture, containing the excess of phenol was

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saturated with dry hydrogen chloride and left for 48 h at room temperature. The crude product was collected by filtration and crystallized several times from toluene.

Spiking experiments of impurities were conducted in a pilot facility for interfacial PC polymerization at 5 kg scale. Five batches were made at each setting.

Results and Discussion

In an initial phase of this study, samples were collected across the bisphenol-A (BPA) monomer plant, the resin plant and the finishing facility.

The BPA plant transforms phenol and acetone into BPA in an acid catalyzed process. The resulting crude mixture of BPA, Phenol and by-products is subjected to a series of purification steps to yield BPA crystals of the required purity.

In the resin plant, BPA and phosgene are reacted in the presence of water and dichloromethane (DCM) while the pH is kept high through the addition of caustic. The result is a mixture containing PC resin dissolved in DCM and brine. The organic solution goes through washing and purification steps and is dried to isolate the PC resin.

Finally the finishing plant extrudes the resin into granulates while adding additives such as heat stabilizers, colorants, UV stabilizers and the like.

A method was developed which allows impurities that are formed during BPA synthesis to be traced back during all stages of making and using the polycarbonate and derived products, according to embodiments. A mild depolymerization procedure destroys carbonate and ester linkages and restores the BPA monomer together with its impurities, which can then be analyzed. The method can be applied to plant streams, resin powder, granulate or molded products including items taken from the market for competitive analyses.

Samples were taken in such a way that monomer, resin and granulate samples would match one another, i.e. the monomer sample would be the one used to make the resin sample and the resin sample would be the material that was used in generating the plastic granulate. Twenty of such sample sets were taken. Every sample was subjected to various tests to determine metal and ion contamination levels, organic purity, polymer end groups, etc. Finally, all of the analytical results were inspected for correlation to the color and transmission of molded plaques of the granulate.

The results of this baseline study are summarized in Table 1, which lists those measured properties, which were found to give a statistically relevant correlation to YI.

Table 1 set forth below discloses sample properties correlated to yellowness index.

TABLE 1

	Initial color	Heat aged color
BPA process	BPX-1, chroman, spirobisindane, BPX-2 DMX BPA organic purity sum of unknowns	, BPX-2 BPA organic purity
Resin process	resin oligomers residual <sup>1</sup> PCP, BPA OH endgroups Cl <sup>-</sup> , Na <sup>+</sup> , Ca <sup>++</sup> , Fe <sup>3+</sup> , Ni <sup>++</sup> , Cu <sup>++</sup> , Zn <sup>++</sup>	resin oligomers residual PCP, BPA ortho OH groups

1para-cumylphenol

Table 2 sets forth below shows the average percent change in organic impurities during plant processes. Only those numbers are reported which are statistically significantly different from zero in the sample set. Species which are constant along the process are not reported therein.

27 TABLE 2

	reaction	extrusion	STD molding	ABU molding	heat ageing
Phenol					+36
IPP	+76				
opBPA			-11	-11	-8
BPX-1			-9	-8	-15
SBI			+53	+59	
BPX-2			-32	-31	
DMX					-54
unknowns	-66		+240	+305	+210

During reaction, the concentration of most impurities does not change. This is also not expected since all of these impurities have at least one para-substituted OH group, which will react in a similar manner as BPA and result in incorporation in the polymer backbone. Besides, if any new impurities are formed during the reaction at low temperature and high pH, it is unlikely that these will have a similar nature as those formed in an acidic environment at high temperatures. Most of the impurities being constant indicates the applicability of this method. IPP (4-isopropenyl phenol) is the only species going up during the resin reaction and unknowns are going down. The latter can be explained by the washing out of unreactive impurities during the resin cleaning steps. During extrusion, no significant changes in impurity levels take place. A more significant heat input is given to the materials during molding. Both during standard and abusive molding the levels of spirobisindane (SBI) and unknowns go up.

SBI is utilized as a monomer for polycarbonates with specific optical properties and enhanced glass transition temperature. Although polymers with high levels of SBI do not have the same color stability as BPA based polycarbonate, this compound is not expected to be a significant factor in 35 discoloration at trace levels. A considerable effort was undertaken in looking at the peaks of individual unknown species, correlating them to color and trying to identify their structure. This has not led to the identification of a color body, unforing and heat aging, it may be interesting to look at what disappears. Both opBPA and BPX-1 are components whose concentration decreases as color increases. In earlier reports opBPA or BPX-1 have never been suspect with regard to discoloration. Their ortho OH groups have been considered 45 mostly harmless.

Based on the results of the correlations (Table 1), as well as the particular profiles of opBPA and BPX-1 along the process (Table 2), it was decided to run a number of polymerization experiments with specific impurities independently spiked in 50 at various concentrations. BPX-1, chroman and DMX were synthesized and isolated for this purpose, opBPA was expected to behave in a comparable manner to BPX-1 due to the similarity of the structure (FIG. 3) and in concentration profile (Table 2) and was not tested. FIG. 3 is a schematic 55 undertaken to work on the overall resin manufacturing proillustration of selected BPA impurities potentially related to

Chroman and DMX were spiked at four levels in the range of 100 to 1,000 ppm relative to BPA. BPX-1 was spiked at 5 levels in the range of 200 to 2,000 ppm. High purity BPA 60 (99.92 wt %) was used for the polymerizations to minimize the effects of other impurities on the final color. Reference samples without any spiked impurity were generated for comparison. The initial color results had YI in the range of 1.5 to 2.0, but none of the variation was correlated to the spiked 65 impurities. The results for the color shift upon 2,000 hours of heat aging are shown in FIG. 4. In particular, FIG. 4 shows

changes in YI after 2,000 hours, heat aging at 130° C. as a function of spiking level of three different impurities (delta YI(-) versus spiking level (ppm).

The profiles for DMX and chroman are flat indicating these species are not related to color stability. However, BPX-1 clearly increases yellowness in the material after aging. This relationship between BPX-1 and color stability only holds if the BPX-1 is spiked in a fixed, high purity BPA. A data point for a sample derived from a regular quality of BPA is plotted 10 at its BPX-1 level of 150 ppm, but clearly there are other components in this sample which further increase the discoloration. A second datapoint based on yet another BPA sample of different quality is placed at 400 ppm and WI of 9.2, off the scale of the graph.

If BPX-1 degradation lies at the root of this discoloration, it can be hypothesized that a scission reaction takes places that splits the BPX-1 unit into a ppBPA unit and an IPP unit and that this IPP unit leads to colored by products. Note that these units are not present in the material in the form in which they are presented in FIG. 3, but have reacted to their carbonate equivalent in-chain units. Likewise, then, opBPA can undergo a scission reaction to give phenol and IPP. Indeed, if all datapoints are plotted as a function of the total level of opBPA and BPX-1 together, then a straight line is found (FIG. 5). FIG. 5 is a graph depicting the change in YI after 2,000 hours, heat aging at 130° C. as a function of the summed level of BPX-1 and opBPA as determined analytically (delta YI versus BPX-1+opBPA (ppm).

Note that the standard quality BPA dataset in this plot is based on samples from three different BPA sources with varying quality levels polymerized at pilot plant and commercial scale in three different facilities. Both samples which have been spiked as well as those in which the opBPA and BPX-1 components are present as the residuals from BPA synthesis fall on the same line, which justifies the conclusion that these species lie at the origin of discoloration during heat aging and are not just correlated to discoloration in a noncausal fashion.

Interestingly, extrapolating the fitted line shows that in tunately. Rather than looking at what is formed during mold- 40 absence of BPX-1 and opBPA, the discoloration would be reduced to WI 0.5, which is only a small fraction of the discoloration observed in the samples derived from regular BPA, meaning that these two components are the main contributors to discoloration.

> Knowing which monomer impurities are detrimental to color stability is a good thing; the downside however is that opBPA is the most prominent impurity that is formed during BPA synthesis and not a component whose formation can be easily prevented in reaction or which is easily reduced in a selective way during in downstream purification steps. Therefore, improving the purification steps for BPA in a general sense proves the more cost effective way of improving resin color stability.

> Besides this work on BPA impurities, further efforts were cess parameters (Table 1) and on formulation and compounding aspects to produce the final granulated product. The advantages of this combined approach become apparent in FIG. 6. FIG. 6 is a graph depicting implementation of the described process improvements combined with an optimized formulation improved the PC grade (delta YI(-) versus time (hours)).

> Improving the manufacturing processes leads to a more sustainable performance gain than what can be achieved through color stabilizing and compensating additives alone. Additives may lose their effectiveness over time as can be seen in the product of 'A', that suddenly develops color in an

accelerated way after 1,000 hours (hrs) of aging. Both our materials as well as the product of 'B' exhibit a predictable aging behavior and with the improvements that we have implemented, our PC products offer state of the art performance.

It has been shown that the major source of color instability lies as early in the manufacturing process as during monomer synthesis. The combined efforts of process improvement and product development have led to products which combine a high light transmission, low color and excellent retention of these properties in heat aging which makes them well suited for applications in which long lifetimes are required such as LED bulbs and lenses and those in which long path lengths are used such as lightguides.

It is noted that the afore-described experimental results regarding Lexan\* polycarbonate is particularly advantageous in that Lexan\* polycarbonate has excellent mechanical properties, which combined with its inherent transparency, make it the material of choice for lighting applications such as lenses, 20 lightguides and bulbs, as well as construction of roofing, greenhouses, verandas, and so forth. With the advent of LED technology, the functional lifetime of lighting products has increased impressively and will further expand in the years to come. Also, in construction application, durability is impor- 25 tant. Plastics will age, however, under the influence of heat, light and time, causing reduced light transmission and color changes. The inventors have herein addressed the above concerns and others, according to embodiments, to explain the factors such as BPA purity level, sulfur level, hydroxy level, type of process employed (interfacial) that can determine the optical material performance. The inventors have advantageously determined how optimization of such parameters during monomer and resin production can lead to further enhancement of color and color stability of the resulting plastic.

As further shown in Table 3, the polymerization type and BPA purity can dictate heat aging color stability. Table 3 depicts YI (2000 hours, 130° C. and BPA purity (%)). A 4 higher purity BPA can lead to 85% reduction of discoloration.

TABLE 3

resin process	BPA organic purity	YI (2000 hrs @ 130° C.)
Interfacial	99.45	13.3
Interfacial	99.51	13.0
Interfacial	99.63	10.7
Interfacial	99.78	7.3
Melt	99.78	15.5
Melt	99.77	16.1
Melt	99.78	19.1

FIG. 7 is an exemplary chemical formula illustrating the formation of BPA; the reaction is catalyzed through either a 55 soluble organic thiol containing acidic compound. (referred to as 'old catalyst' or an insoluble resin with acidic and thiol functionality which is insoluble in BPA and the reaction mixture of BPA synthesis.

The catalyst can be attached to an insoluble resin for the 60 reduction of sulfur in BPA, e.g., down to less than 0.5 ppm, which resulted in a significant reduction in YI (e.g., from greater than 1.4, specifically up to 1.8, down to less than 1.4 and even down to 1.2).

FIG. 9 is a bar graph comparing the yellowness index (YI) 65 for an exemplary polycarbonate (LEXAN\* polycarbonate grade PC175 having a melt volume rate of 30) with the bulk

catalyst (bars "A"), the attached catalyst (bars "B"), and with the attached catalyst and a BPA purity of 99.65 wt % (bar "C").

FIG. 10 is a bar graph comparing the yellowness index (YI) for an exemplary polycarbonate (LEXAN\* polycarbonate grade PC105 having a melt volume rate of 6) with the bulk catalyst (bars "A"), the attached catalyst (bars "B"), and with the attached catalyst and a BPA purity of 99.65 wt % (bars "C").

FIG. 11 shows a comparison of the yellowness index (YI) for an exemplary polycarbonate (LEXAN\* polycarbonate grade PC135 having a melt volume rate of 4) with the attached catalyst (bars "B"), and with the attached catalyst and a BPA purity of 99.65 wt % (bars "C").

FIG. 12 is a graphical illustration of change in YI over time for various grades of LEXAN\* polycarbonate formed with the new catalyst or with the new BPA using a free hydroxyl concentration of less than 150 ppm.

Table 4 shows the various formulations tested. Resin was compounded with various heat stabilizers at two different levels each. The dependency of initial color, color stability in heat aging and hydrolitic stability (molar mass stability in autoclaving) on additive concentration was evaluated and rated quantitatively as ++ (highly desirable), + (desirable), O (neutral), - (undesirable), -- (highly undesirable).

TABLE 4

Initial YI	HA YI**	HYDROLIC STABILITY	MVR CHANGE
+	+	+	+
+	+	-	+
+	0	-	+
+	+	-	+
+	_	-	+
++	0	+	+
-	_	_	+
+	_	_	+
+	+	0	+
+	-	+	+
_	_	-	+
_	_	+	+
	+ + + +	+ + + + + 0 + + +	Initial YI

<sup>&</sup>lt;sup>1</sup>Tris (2,4-di-ert-butylphenyl)phosphite

As noted above, HPLC (high performance liquid chromatography or high pressure liquid chromatography) can be used to determine BPA purity. Set forth below are further details, according to embodiments.

## Sample Preparation:

About 200 milligrams (mg) of the sample is weighed accurately. It is dissolved in 5 ml of tetrahydrofuran (THF) and 2 ml of a 10% solution of potassium hydroxide diluted in methanol. The depolymerization of polycarbonate is carried out with the use of these solvents.

The solution is shaken for 2 hours. Then, 2 milliliters (ml) of acetic acid are added to protonate the BPA carbonate salts

<sup>&</sup>lt;sup>2</sup>Dioleyl hydrogen phosphite commercially available from Dover Chemical, Dover, Ohio <sup>3</sup>4-[4-bis(2,4-ditert-burylphenoxy)phosphanylphenyl]

<sup>&</sup>lt;sup>4</sup>bis(2,4-di-t-butyphenyl)pentraerythritol diphosphite commercially available from Chemtura Corporation, Middlebury, CT <sup>3</sup>tris(nonylphenyl)phosphite

<sup>6</sup>triphenyl phosphine

diphenyl isodecyl phosphite

<sup>&</sup>lt;sup>8</sup>octadecyl3(3,5ditertbutyl4hydroxyphenyl)propionate commercially available from Chemtura Coporation pentaerythritol-tetrakis(3(3,5-di-tert.butyl-4-hydroxy-phenyl-)propionate) commercial-

openaerymritor-terrakis(3,5,3-cit-tert.outy)-4-nydroxy-pnenyi-,propionate) commerciallyavailable from Chemtura Corporation 10bis(2,2,6,6-tetramethyl-4-piperidyl)sebacate

<sup>&</sup>lt;sup>11</sup>phenolic antioxidant N,N-hexane-1.6-diylbis[3-(3,5-di-tert-butyl-4 hydroxyphenylepropionamide)]

<sup>\*</sup>tested on combination with 500 ppm Igrafos 168

<sup>\*\*</sup>based upon 750 hours at 130° C.

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and decrease the pH. The solution is shaken again for half an hour for homogenization and dissolution of all precipitates. Standard Sample Preparation:

These samples containing only one impurity determine the retention time and the calibration coefficient of each impurity. The impurity is dissolved in 10 ml of methanol. The mass is calculated in order to obtain a concentration in vial between 50 and 100 ppm. One ml of this solution is taken and diluted in 10 ml of methanol.

All the different solutions are put in vials by the aid of a syringe with a filter. For both impurities and samples, a blank is made in order to explain a strange peak or a problem in the solvent. The blank has the same solvent composition as the sample. It means that for the standard sample the blank contains only methanol. For the samples, the blank corresponds to a mix of 5 ml of THF, 2 ml of Methanol and 2 ml of Acetic Acid.

# Experiments:

The device used for the HPLC analysis is an Agilent 1100 system. The software used is Agilent ChemStation. The <sup>20</sup> analysis is carried out on a C18 column. A gradient of polar solvents is used. It is a mixture of water and methanol. THF is used at the end of the analysis to clean the column. Table 5 sets forth the solvent gradient profile.

TABLE 5

Time (min)	$\begin{array}{l} {\rm H_2O} + 0.1\% \\ {\rm H_3PO_3}\left(\%\right) \end{array}$	MeOH (%)	THF (%)
7	60	40	0
31	10	90	0
33	0	60	40
34	0	60	40
35	60	40	0
44	60	40	0

The applied flow is 1.2 milliliters per minute (ml/min). The output is recorded as a series of peaks, each one representing a compound. All peaks are integrated on the chromatogram to obtain the peak area. For all impurities except for DMX, the integration is done at 280 nm. For the DMX, the integration is performed at 254 nm because the peak is more visible. To identify each peak, the retention time can be used but with caution because in function of the conditions the retention time can change (pressure, solvent, column, temperature . . . ). Table 6 summarizes the different studied impurities (impurities contained in PC with their corresponding retention times).

TABLE 6

Impurity	Retention time (min)	
Phenol	2.44	
IPP	7.49	
ppBPA	10.69	55
opBPA	14.66	
1CD2	17.32	
<sup>2</sup> CD1	18.49	
PCP	18.98	
BPX 1	20.20	
Chroman 1	20.66	60
Chroman 1,5	22.49	
SBI	23.38	
BPX 2	24.11	
DMX (254 nm)	24.58	

 $<sup>^1\</sup>rm cyclic$  dimer-2, a1H-Inden-5-ol, 2,3-dihydro-1-(4-hydroxyphenyl)-1,3,3-trimethyl-  $^2\rm a$  cyclic dimer of isopropenylphenol 1H-Inden-5-ol, 2,3-dihydro-3-(4-hydroxyphenyl)-1,

Determination of the Impurities Concentration in Polycarbonate:

The impurities concentration in polycarbonate is found from the chromatograms analysis. Then, the BPA purity can be deduced. Using the area corresponding to the retention time for impurities, the impurities concentration in the vial can be calculated. For that, the area of each peak is multiplied by 1,000 to obtain a concentration in milligrams per liter (mg/L) of each impurity in the vial. Then, it is divided by each impurity calibration coefficient.

concentration of impurity (vial) = 
$$\frac{\text{peak area} * 1000}{\text{calibration coefficient}}$$

From the accurate amount weighted at the beginning for each sample, the initial concentration of the vial is calculated in mg/L.

The concentration of impurities in polycarbonate is determined by multiplying the concentration of impurities in the vial by 1,000,000 in order to convert the concentration in ppm. Then, this result is divided by the concentration of the sample.

concentration of impurity (PC) =

 $\frac{\text{concentration of impurity (vial)}*1000000}{\text{sample concentration}}$ 

Determination of the Impurities Weight Percentage in PC:

The areas of unknown peaks that appear before the DMX peak are summed. The concentration of unknowns is determined by using the BPX-2 coefficient. The use of this coefficient was chosen arbitrarily. All the concentrations of known and unknown impurities (except BPA, phenol and PCP) are added. The concentration found in parts per million (ppm) is transformed to wt % by dividing by 10,000. Like that, the wt % of impurities is found in the resin.

wt % of impurities = 
$$\frac{\sum Concentration of impurities}{10000}$$

BPA Purity Determination:

After, a coefficient is applied to determine the wt % of impurities in BPA. The samples are weighted before depolymerization. The BPA molar mass is different from the carbonated BPA. For that, we multiply by 254 grams per mole (g/mol) and divide by 228 g/mol. 254 g/mol corresponds to the resin molar mass and the BPA molar mass is equal to 228 g/mol.

wt % of impurities in 
$$BPA = \frac{\text{wt \% of impurities} * 254}{228}$$

BPA (M = 228 g/mol)

$$\begin{array}{c} \text{-continued} \\ \text{CH}_3 \\ \\ \text{H}_3 \\ \end{array} \\ \begin{array}{c} \text{O} \\ \\ \end{array} \\ \begin{array}{c} \text{O} \\ \\ \\ \end{array} \\ R \end{array}$$

carbonated BPA (M = 254 g/mol)

The BPA purity is determined by subtracting the wt % of impurities in initial BPA from 100. BPA purity=100-% wt of  $^{10}$  impurities in BPA.

In an embodiment, a composition comprises: bisphenol-A polycarbonate, wherein a molded article of the composition has transmission level greater than or equal to 90.0% at 2.5 mm thickness as measured by ASTM D1003-00 and a yellow index (YI) less than or equal to 1.5 as measured by ASTM D1925. In an embodiment, an article comprises the composition

An embodiment of a method of making a polycarbonate composition comprises: polymerizing by an interfacial polymerization, reactants comprising a starting material comprising a bisphenol-A having a purity of greater than or equal to 99.65 wt % and a sulfur content of less than or equal to 2 ppm, wherein the polycarbonate composition has a free hydroxyl content of less than or equal to 150 ppm, and wherein a molded article of the polycarbonate composition has transmission level greater than or equal to 90.0% at 2.5 mm thickness as measured by ASTM D1003-00 and a yellow index (YI) less than or equal to 1.5 as measured by ASTM D1925.

In the various embodiments, (i) the bisphenol-A polycarbonate can comprise less than or equal to 150 ppm free hydroxyl groups; and/or (ii) the bisphenol-A polycarbonate comprises sulfur in an amount less than or equal to 2 ppm sulfur; and/or (iii) the molded article comprises an increase in 35 yellow index (YI) of less than 2 during 2,000 hours of heat aging at 130° C.; and/or (iv) the bisphenol-A polycarbonate is an interfacially polymerized polycarbonate; and/or (v) further comprising a flame retardant; and/or (vi) further comprising a second polycarbonate derived from bisphenol-A, 40 wherein the second polycarbonate is different than the bisphenol-A polycarbonate; and/or (vii) further comprising a second polycarbonate, wherein the second polycarbonate is selected from at least one of the following: a homopolycarbonate derived from a bisphenol; and/or (viii) a copolycar- 45 bonate derived from more than on bisphenol; and a copolymer derived from one or more bisphenols and comprising one or more aliphatic ester units or aromatic ester units or siloxane units; and/or (ix) further comprising one or more additives selected from at least one of the following: UV stabilizing 50 additives, thermal stabilizing additives, mold release agents, colorants, organic fillers, inorganic fillers, and gamma-stabilizing agents; and/or (x) the article is selected from at least one of the following: a light guide, a light guide panel, a lens, a cover (e.g., LED cover), a sheet, a bulb, and a film; and/or 55 (xi) the article is a LED lens; and/or (xii) the article comprises at least one of the following: a portion of a roof, a portion of a greenhouse, and a portion of a veranda; and/or (xiii) further comprising dissolving a reactant in an aqueous caustic material, adding the resultant mixture to a solvent medium, and 60 contacting the reactants with a carbonate precursor in presence of a catalyst; and/or (xiv) using an end-capping agent (e.g., endcapping the polycarbonate); and/or (xv) the endcapping agent can be selected from at least one of the following: phenol or a phenol containing one or more substitutions 65 with at least one of the following: aliphatic groups, olefinic groups, aromatic groups, halogens, ester groups, and ether

groups; and/or (xvi) the end-capping agent can be selected from at least one of the following: phenol, p-t-butylphenol, and p-cumylphenol; and/or (xvii) the method can exclude use of a melt polymerization process to make the polycarbonate. Also included herein are articles formed by any of the above methods.

It is noted herein that all weight percents do not exceed 100 wt %.

Also, all ranges disclosed herein are inclusive of the endpoints, and the endpoints are independently combinable with each other, and inclusive of all intermediate values of the ranges. Thus, ranges articulated within this disclosure, e.g. numerics/values, shall include disclosure for possession purposes and claim purposes of the individual points within the range, sub-ranges, and combinations thereof.

Reference throughout the specification to "one embodiment", "another embodiment", "an embodiment", and so forth means that a particular element (e.g., feature, structure, and/or characteristic) described in connection with the embodiment is included in at least one embodiment described herein, and may or may not be present in other embodiments. In addition, it is to be understood that the described elements may be combined in any suitable manner in the various embodiments. Various combinations of elements of this disclosure are encompassed by the embodiments disclosed herein, e.g. combinations of elements from dependent claims that depend upon the same independent claim.

The suffix (s) as used herein is intended to include both the singular and the plural of the term that it modifies, thereby including one or more of that term (e.g., the colorant(s) includes one or more colorants).

In general, the compositions or methods may alternatively comprise, consist of, or consist essentially of, any appropriate components or steps herein disclosed. The invention may additionally, or alternatively, be formulated so as to be devoid, or substantially free, of any components, materials, ingredients, adjuvants, or species, or steps used in the prior art compositions or that are otherwise not necessary to the achievement of the function and/or objectives of the present claims

As used herein, "combination" is inclusive of blends, mixtures, alloys, reaction products, and the like.

All cited patents, patent applications, and other references are incorporated herein by reference in their entirety. However, if a term in the present application contradicts or conflicts with a term in the incorporated reference, the term from the present application takes precedence over the conflicting term from the incorporated reference.

While particular embodiments have been described, alternatives, modifications, variations, improvements, and substantial equivalents that are or may be presently unforeseen may arise to applicants or others skilled in the art. Accordingly, the appended claims as filed and as they may be amended are intended to embrace all such alternatives, modifications, variations, improvements, and substantial equivalents.

#### What is claimed is:

1. A composition comprising: bisphenol-A polycarbonate, wherein a molded article of the composition has transmission level greater than or equal to 90.0% at 2.5 mm thickness as measured by ASTM D1003-00, a yellow index (YI) less than or equal to 1.5 as measured by ASTM D1925, and an increase in yellow index of less than 2 during 2,000 hours of heat aging at 130° C., wherein the bisphenol-A polycarbonate comprises less than or equal to 150 ppm free hydroxyl groups and has a sulfur content of less than 2 ppm.

- 2. The composition as in claim 1, wherein the bisphenol-A polycarbonate is an interfacially polymerized polycarbonate.
- 3. The composition as in claim 1, wherein the composition comprises a flame retardant.
- **4**. The composition as in claim **1**, further comprising a second polycarbonate derived from bisphenol-A, wherein the second polycarbonate is different than the bisphenol-A polycarbonate.
- 5. The composition as in claim 1, further comprising a second polycarbonate, wherein the second polycarbonate is selected from at least one of the following: a homopolycarbonate derived from a bisphenol; a copolycarbonate derived from more than one bisphenol; and a copolymer derived from one or more bisphenols and comprising one or more aliphatic ester units or aromatic ester units or siloxane units.
- **6**. The composition as in claim **1**, further comprising one or more additives selected from at least one of the following: UV stabilizing additives, thermal stabilizing additives, mold release agents, colorants, organic fillers, inorganic fillers, and gamma-stabilizing agents.

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- 7. An article comprising the composition of claim 1.
- 8. The article as in claim 7, wherein the article is selected from at least one of the following: a light guide, a light guide panel, a lens, a cover, a sheet, a bulb, and a film.
- 9. The article as in claim 8, wherein the article is a LED lens.
- 10. The article as in claim 7, wherein the article comprises at least one of the following: a portion of a roof, a portion of a greenhouse, and a portion of a veranda.
- 11. The composition of claim 1, wherein the bisphenol-A polycarbonate is an interfacially polymerized polycarbonate derived from bisphenol-A having a purity of greater than or equal to 99.65 wt %.
- 12. The composition of claim 1, wherein the bisphenol-A5 polycarbonate is a homopolycarbonate derived from bisphenol-A.
  - 13. The composition of claim 12, wherein the bisphenol-A polycarbonate is a linear homopolycarbonate derived from bisphenol-A.

\* \* \* \* \*